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# PLANTWIDE CONTROL STRUCTURES DESIGN PROCEDURE APPLIED TO THE HYDRODEALKYLATION PROCESS USING FIXTURE POINT THEOREM

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A Thesis Submitted in Partial Fulfillment of the Requirements
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สุชาดา สันติศรีโกมล : วิธีการออกแบบโครงสร้างการควบคุมแพลนท์ไวด์ของกระบวนการไฮโดรดีอัลคิลเลชันโดยทฤษฎีจุดตรึง. (PLANTWIDE CONTROL STRUCTURES DESIGN PROCEDURE APPLIED TO THE HYDRODEALKYLATION PROCESS USING FIXTURE POINT THEOREM)
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กระบวนการทางเคมีที่มีความซับซ้อน เช่น กระบวนการที่มีการนำมวลสาร และพลังงานกลับมาใช้ใหม่เพื่อให้เกิดความคุ้มค่ามากที่สุด มีผลทำให้การออกกระบวนการมีความซับซ้อนมากขึ้น การออกแบบลูพควบคุมกระบวนการให้เหมาะสมมีผลต่อภาวะการดำเนินงานที่ดี

ในงานวิจัยนี้ได้นำเสนอการออกแบบโครงสร้างการควบคุมจากปัญหาทั่วไปของการออกแบบโครงสร้างการควบคุมคือการเลือกชุดของตัวแปรควบคุมที่เหมาะสมจับคู่กับตัวแปรปรับเพื่อให้ได้ลูพโครงสร้างการควบคุมที่ดี ที่สามารถกำจัดความแปรปรวนที่เกิดขึ้นในระบบได้อย่างรวดเร็ว ในงานวิจัยนี้ได้เสนอแนวคิดวิธีการเลือกชุดของตัวแปรควบคุม โดยเลือกตัวแปรที่เมื่อเกิดการเปลี่ยนแปลงแล้วส่งผลกระทบต่อกระบวนการมากที่สุดและมีความไวมากที่สุดเมื่อมีความแปรปรวนเข้าสู่ระบบ เพื่อที่จะสามารถกำจัดความแปรปรวนที่เกิดขึ้นในระบบได้อย่างรวดเร็ว ทฤษฎีนี้เรียกว่า "ทฤษฎีจุดตรึง" (Fixture point theorem) วิธีการนี้จะให้อันดับของความสำคัญของตัวแปรที่มีผลต่อกระบวนการและอาศัยผล(สเกล)เกนสูงสุดในการเลือกจับคู่ตัวแปรควบคุมและตัวแปรปรับที่เหมาะสมโดยเลือกจับคู่ตามอันดับความสำคัญของตัวแปรที่ได้ ผลการวิจัยพบว่าชุดของตัวแปรควบคุมที่มีผลต่อกระบวนการมากที่สุดคล้ายกับชุดของตัวแปรที่ได้จากประสบการณ์ของLuyben(1998) วิธีการออกแบบที่ได้เสนอนี้ เป็นวิธีพื้นฐานที่เข้าใจง่าย และให้ผลดี งานวิจัยนี้ได้ทำการเลือกชุดของตัวแปรควบคุมสามชุดตัวแปร และออกแบบโครงสร้างการควบคุมทั้งหมด 5 โครงสร้างเพื่อเปรียบเทียบ ในการแสดงพฤติกรรมเชิงพลวัตรของการออกแบบโครงสร้างควบคุมแบบแพลนท์ไวด์ของกระบวนการไฮโดรดิแอลคิลเลชันโดยสร้างการรบกวนระบบคือ เปลี่ยนสัดส่วนของมีเทน และอุณหภูมิขาเข้าเครื่องแลกเปลี่ยนความร้อน ซึ่งพบว่าโครงสร้างการควบคุมที่ออกแบบด้วยวิธีนี้ ให้ค่าเวลาความคลาดเคลื่อนแบบสมบูรณ์และปริมาณการผลิตผลิตภัณฑ์ มีค่าใกล้เคียงกับโครงสร้างการควบคุมอ้างอิงที่2 (Luyben,1998) และมีความเบี่ยงเบนน้อยกว่าโครงสร้างการควบคุมอ้างอิงที่1 (Araujo,2006)

ภาควิชา.......วิศวกรรมเคมี.............. ลายมือชื่อนิสิต...สุชาดา สันติศรีโกมล...........
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KEYWORDS : HDA PROCESS/ PLANTWIDE PROCESS CONTROL/ FIXTURE POINT THEOREM/ SELECTION OF CONTROLLED VARIABLE.

SUCHADA SUNTISRIKOMOL: PLANTWIDE CONTROL STRUCTURES DESIGN PROCEDURE APPLIED TO THE HYDRODEALKYLATION PROCESS USING FIXTURE POINT THEOREM. ADVISOR: ASST.PROF. MONTREE WONGSRI, D.Sc., 151 pp.

Design a process control structure for a complex process, such as the process having material or energy recycle, is a complicate task. The design control loop would effect the operation significantly.

This thesis describes the plantwide control structure design procedure base on general problem that are "what variables should be control" and "How to design the control configuration", the Hydrodealkylation process (HDA) for case study; hence, we present the "Fixture point theorem" to select appropriate the set of controlled variables from a large number of candidate output. The fixture point control theorem states that the most disturbed points must be satisfactorily controlled by giving them consideration before other controlled variables. The maximum (scaled) gain is used to selecting and paring controlled variables with manipulated variables. In this study, the set of first rank of controlled variables is the same as Luyben (1998). We selected three set of controlled variables (second and third rank from fixture point) and five control structures were designed and compared. In order to illustrate the dynamic behaviors of the control structures when economic disturbance load occur such as change in methane composition in fresh feed gas and quencher outlet temperature. The performance of designed control structures were presented in IAE value and compared with reference structure. The designed structures are fast response and the most effective on compared with reference structure1 (Araujo et al, 2006) and same reference structure 2 (Luyben, 1998).

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# CHAPTER I

# INTRODUCTIONS

This Chapter is an introduction of this research. It consists of importance and reasons for research, research objective, scope of research, contribution of research and research contents.

## 1.1 Importance and Reasons for research

Control structure design deals with the structural decisions of control system, including what to control and how to pair the variables to the best set of form control loop. Although these are very important issues, these decisions are in most case made in a fashion, base on experience and engineering insight, without considering the details of process variable link with problem.

The general problems of plantwide control design procedure are selection the controlled variables, selection the manipulated variables, selection the measurement, pairing the controlled and manipulated variables for the best control configurations and selection of controller type.

The process had good controllability one reason came from selection appropriate the set of controlled and manipulated variables for the control configuration of chemical plant.

In this paper propose a basic idea of fixture point control is used for screening controlled variable and paring with manipulated variable.

Hydrodealkylation (HDA) process is widely used because it is a realistically complex chemical process that creates disturbance propagation and the complicated system's dynamic behavior. Therefore, this research will design plantwide control structures of Hydrodealkylation (HDA) process using new plantwide control structure design procedure to select set of controlled variables and simulate them by using HYSYS simulator in order to study about dynamic behavior and evaluate the performance of the designed structures.

## 1.2 Research Objective

The objectives of this research are:

1. To simulate Hydrodealkylation (HDA) of toluene process both steady state and dynamics condition by using HYSYS simulator.
2. To design plantwide control structures of Hydrodealkylation (HDA) process using Fixture point theorem (Wongsri, 2008).

## 1.3 Scopes of research

The scope of this research can be listed as follows:

1. The simulator in this research is HYSYS simulator.

2. Description and data of Hydrodealkylation (HDA) process is obtained from Douglas, J. M.(1998), William L. Luyben, Bjorn D. Tyreus, and Michael L. Luyben (1998), William L. Luyben (2002) and Araujo et al,(2006).

3. To design 3 control structures of Hydrodealkylation (HDA) process.

## 1.4 Contributions of research

The expected contribution of this research is:

This research provides the appropriate controlled variables and good efficacious design control structure by using new plantwide control structure design procedure.

## 1.5 Research procedures

Procedure plans of this research are:

1. Study of general plantwide control structure design procedure.

2. Study of Hydrodealkylation (HDA) process and concerned information.

3. Simulations of the Hydrodealkylation (HDA) process at steady state and dynamic.

4. Screening key process variables for fixture point analysis (Only reaction section).

5. Pairing manipulated variable with control variables of Hydrodealkylation (HDA) process.

6. Simulation of the Hydrodealkylation (HDA) process at dynamic.

7. Collection and summarization of simulation results.

## 1.6 Research Framework

This thesis matter is classified into six chapters as follows:

| | |
|---|---|
| **Chapter I** | provides an introduction, motivation, objectives, scopes, contributions and thesis outline. |
| **Chapter II** | presents literature review related to plantwide control structure design procedure and the method of selection set of controlled variables. |
| **Chapter III** | purpose new plantwide control structure design procedure and present the fixture point theorem for selection appropriate set of controlled variables. |
| **Chapter IV** | shows case study of the Hydrodealkylation process (HDA) by using theory in chapter 3. |
| **Chapter V** | shows control structure alternatives. |
| **Chapter VI** | the last chapter shows overall conclusions of this research and recommendations for future research. |

This is followed by:
Appendix A: Tuning of Control structures
Appendix B: Parameter Tuning
Appendix C: Data of fixture point analysis
Appendix D: HDA process flowsheet with controller installed
Appendix E: Graph of dynamic response

# CHAPTER II

# LITERATURE REVIEW

## A. Plantwide control design procedure

### 2.1 Heuristics- Approach Base

#### 2.1.1 Hierarchical decomposition based on process structure

The hierarchy given in Douglas (1988) for process design starts at a crude representation and gets more detailed:

Level 1: Bath vs continuous
Level 2: Input-output structure
Level 3: Recycle structure
Level 4: General structure of separation system
Level 5: Energy interaction

Fisher et al. (1988) propose to use this hierarchy when performing controllability analysis, and Ponton and Laing (1993) point out that this hierarchy, (e.g. level 2 to level 5) could also be used for control system design.

Ng and Stephanopoulos (1998b) propose to use a similar hierarchy for control structure design. The difference between Douglas (1988) and Ng and Stephanopoulos (1998b)'s hierarchy is that level 1 is replaced by a preliminary analysis and that levels 4 and 5 are replaced by more detailed structures. At each step the objectives identified at an earlier step is translated to this level and new objectives are identified. The focus is on construction of mass and energy balance control. The method is applied to the Tennessee Eastman case.

All these methods have in common that at each step (level), a key point is to check if there remain enough manipulated variables to meet the constrains and to optimize operation.

### 2.1.2 Hierarchical decomposition based on control objectives

The hierarchy based on control objectives is sometime called the tiered procedure. This bottom-up procedure focuses on the task that the controller has to perform. Normally one starts by stabilizing the plant, which mainly involves placing inventory (mass and energy) controllers.

Price et al. (1993) build on the idea that was introduced by Buckley (1964) and introduce a tiered framework. The framework is divided into four different tasks:

I Inventory and production rate control
II Product specification control
III Equipment & operating constraints
IV Economic performance enhancement

Their paper does not discuss points III or IV. They perform a large number of simulations with different control structures, controllers (P or PI), and tunings on a simple process consisting of a reactor, separator and recycle of unreacted reactant. The configurations are ranked based on integrated absolute error of the product composition for steps in the disturbance. From this simulation they propose some guidelines for selecting the though-put manipulator and inventory controls (1) Prefer internal flows as through-put manipulator. (2) The though-put manipulator and inventory controls should be self-consistent (self-consistent id fulfilled when a change in the though-put propagation through the process by itself and does not depend on composition controllers). They apply their ideas on the Tennessee Eastman problem (Price et al.1994).

Ricker (1996) comments on the work of Price et al. (1994) and points out that plant is often run at full capacity, corresponding to constraints in one or several variables. If a manipulated variable used for level control structures, one looses a degree of freedom for maximum production. This should be considered when choosing a though-put manipulator.

Luyben et al. (1997) point out three limitations of the approach of Buckley. First, he did not explicitly discuss energy management. Second, he did not look at recycles.

Third, he placed emphasis on inventory control before quality control. Their plantwide control design procedure is listed below:

1. Establish control objectives.
2. Determine the control degrees of freedom by counting the number of independent valves.
3. Establish energy inventory control, for removing the heats of reactions and to prevent propagation of thermal disturbances.
4. Set production rate. The production rate can only be increased by increasing the reaction rate in the reactor. One recommendation is to use the input to separation section.
5. Product quality and safety control. Here they recommend the usual ‘pair close’ rule.
6. Inventory control. Fix a flow in all liquid recycle loops. They state that all liquid levels and gas pressure should be controlled.
7. Check component balances. (After this point it might be necessary to go back to item 4).
8. Unit operations control.
9. Use remaining control degree of freedom to optimize economics or improve dynamic controllability.

They apply their procedure on several test problems; the vinyl acetate monomer process, the Tennessee Eastman process, and the HDA process.

Step 3 comes before determining the throughput manipulator, since the reactor is typically the heart of the process and the method for heat removal are intrinsically part of the reactor design. In order to avoid recycling of disturbances they suggest to set a flowrate in all recycle loops; they suggest in step 6 to control all inventories, but this may not be necessary in all case; e.g. it may be optimal to let the pressure float (Shinskey 1988). Skogestad et al. (2000) recommend combining step 1 and 9, that is, the selection of controlled variables (control objectives) in step 1 should be based on overall plant economics.

McAvoy (1999) presents a method where the control objectives are divided into two categories: variables that ‘must’ be controlled, and product flow and quality. His approach is to identify the set of inputs that minimizes valve movements. This is first solved for the ‘must’ variables, then for product rate and quality. The optimization problem is simplified by using a linear stable state model. He gives no guidance into how to identify the controlled variables.

### 2.1.3 Hierarchical decomposition based on time scales

Buckley (1964) proposed to design the quality control system as high-pass filters for disturbances and to design the mass balance control system as low pass filters. If the resonance frequency of the quality control system is designed to be order of magnitude higher than the break frequency of mass balance system then the two loops will be non-interacting.

McAvoy and Yc (1994) divide their method into four stages:

1. Design of inner cascade loops.
2. Design of basic decentralized loops; expect those associated with quality and production rate
3. Production rate and quality controls.
4. Higher layer controls

The decomposition in stages 1-3 is based on speed of the loops. In stage 1 the idea is to locally reduce the effect of disturbances. In stage 2 there generally are a large number of alternative configurations. These may be screened using simple controllability tools, such as the RGA. One problem of selecting outputs based on a controllability analysis is that one may end up with the outputs that are easy to control, rather than the ones that are important to control. The method applied to the Tennessee Eastman test problem.

Douglas (1988) presents a hierarchy for control system design, based on steady-state, normal dynamic response and abnormal dynamic operation. Zheng et al. (1999) continue this work and place a greater attention on feasibility in face of constraints and on robust optimality (self-optimizing control). Zheng and Mahajannam (1999) propose to use minimum surge capacity as a dynamic cost.

## 2.2 Mathematical-Approach Base

A chemical plant may have thousands of measurement and control loops. There are some methods that use structural information about the plant as a basis for control structure design. Based on sets of inputs and measurements are classified as viable or non-viable. Although the structural methods are interesting, they are not quantitative and usually provide little information other than confirming insights about the structure of the process that most engineers already have.

The tasks of control structure consist of (1) selection of controlled variables, (2) selection of manipulated variables, (3) selection of measurements and (4) selection of control configuration.

Morari et al (1980), Skogestad and Postlethwaite (1996) and Skogestad (2000) propose to base the selection of controlled variables based on considering the overall operational objective. The overall objective may be formulated as a scalar cost function which should be minimized subject to set of operational constraints.

Morari et al. (1980) propose the basic idea of self-optimizing control propose to select the best set of controlled variables based on minimizing the loss. Skogestad et al (2000) attempt to synthesis a feedback optimizing control structure (self-optimizing control), their main objective is to translate the economic objectives into process control objectives. In other words, they want to find a function c (controlled variables) of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables and optimal operating conditions. This means that by keeping the function $c(u,d)$ at the setpoint $c_s$, through the use of the manipulated variables $u$, for various disturbances $d$, it follows uniquely that the process is operating at the optimal steady-state.

Skogestad (2000) gives four requirements that a controlled variable should meet:

1. Its optimal value should be insensitive disturbance.
2. It should be easy to measure and control accurately.
3. Its value should be sensitive to changes in the manipulated variables.
4. For cases with two or more controlled variables, the selected variables should not be closely correlated.

Yi and Luyben (1995) have studied unconstrained problems, and some of their ideas are related to self-optimizing control. However, Luyben propose to select controlled variables which minimizes the steady-state sensitivity of the manipulated variables $(u)$ to disturbances, i.e. to select controlled variables $(c)$ such that $(\partial u/\partial d)_c$ is small, whereas one should really minimize the steady-state sensitivity of the economic loss $(L)$ to disturbances, i.e. to select controlled variables $(c)$ such that $(\partial L/\partial d)_c$ is small.

## B. Previous work on the HDA process

Stephanopoulos (1984) followed the approach proposed by Buckley (1964) based on material balance and product quality control. He used an HDA plant model where steam is generated from effluent of the feed-effluent heat exchanger through a series of steam coolers. From the material balance viewpoint, the selected controlled variables of choice were fresh toluene feed flow rate (production rate control), recycle gas flow rate , hydrogen content in the recycle gas, purge flow rate, and quencher flow rate. Product quality is controlled through product compositions in the distillation columns and the controlled variables selected are product purity in benzene column and reactor inlet temperature.

Brognaux (1992) implemented both a steady-state and dynamic model of the HDA plant in Speedup$^{TM}$ based on the model developed by Douglas (1988) and used it as an example to compute operability measurements, define control objectives and perform controllability analysis. He found that it is optimal to control the active constraints found by optimization.

Ng and Stephanopoulos (1996) used the HDA process to illustrate how plantwide control systems can be synthesized based on a hierarchical framework. The selection of controlled variables is performed somehow heuristically by prioritizing the implementation of the control objectives. In other words, it is necessary to control the material balances of hydrogen, methane and toluene, the energy balance is controlled by the amount of energy added to the process (as fuel in the furnace, cooling water and steam), production rate and product purity.

Cao, Rossiter and Owens (1997b) considered input and output selection for control structure design proposes using the SVD. Cao, Rossiter and Owens (1998) applied a branch and bound algorithm based on local (linear) analysis.

Ponton and Laing (1993) presented a unified heuristic hierarchical approach to process and control system design based on the ideals of Douglas (1988) and used the HDA process throughout. The controlled variables selected at each stage are: toluene flow rate, hydrogen concentration in the reactor, and methane contents in the compressor inlet (feed product rate control stage): separator liquid stream outlet temperature and toluene contents at the bottom of the toluene column (recycle structure, rates and compositions stage); and separator pressure, benzene contents at stabilizer overhead, and toluene contents at benzene column overhead are related to product and intermediate stream composition stage. The stages related to energy integration and inventory regulation do not cover the HDA process directly, so no controlled variable are assigned at these stages.

Ng and Stephanopoulos (1996) used the HDA process to illustrate how plantwide control systems can be synthesized based on a hierarchical framework. The selection of controlled variables is performed somehow heuristically by prioritizing the implementation of the control objective. In other words, it is necessary to control the material balances of hydrogen, methane and toluene, the energy balance is controlled by the amount of energy added to the process (as fuel in the furnace, cooling water, and stream), production rate and product purity.

Luyben, Tyreus and Luyben (1998) applied a heuristic nine-step procedure together with dynamic simulations to the HDA process and concluded that control performance is worse when the steady-state economic optimal design is used. They chose to control the inventory of all component in the process (hydrogen, methane, benzene, toluene, diphenyl) to ensure that the component material balance are satisfied: the temperature around the reactor are controlled to ensure exothermic heat removal from the process: total toluene flow or reactor inlet temperature (it is not exact) clear which one was selected) can be used to set production rate and product purity by the benzene contents in the benzene column distillate.

Konda, Rangaiah and Krishnaswamy (2005) used an integrated framework of simulation and heuristics and proposed a control structure for the HDA process. They selected fresh toluene feed flow rate to set production rate, product purity at benzene column distillate to fulfill the product specification, overall toluene conversion in the reactor to regulate the toluene recycle loop, ratio of hydrogen to aromatics and quencher outlet temperature to fulfill process constraint, and methane contents in the purge stream to avoid its accumulation in the process.

Antonio, Marius and Sigurd Skogestad (2006) followed the approach proposed by Skogestad (2000) based on Self-optimizing control for selected set of controlled variable. Self-optimizing control is when an acceptable (economic) loss can be achieved using constant set points for the controlled variables, without the need to reoptimize when disturbances occur. They used an HDA process model and SQP algorithm in Aspen Plus$^{TM}$ to find primary controlled variables. They found that it is optimal to specify six variables for distillation columns trade-off between energy usage and recovery:

Stabilizer column: $x_{D,benzene} = 1\times10^{-4}$

$x_{B,methane} = 1\times10^{-6}$

Benzene column: $x_{D,benzene} = 0.9997$ (Active constraint)

$x_{B,benzene} = 1.3\times10^{-3}$

Toluene column: $x_{D,diphenyl} = 5\times10^{-2}$

$x_{B,toluene} = 4\times10^{-2}$

They have five active constraints at reaction section: quencher outlet temperature = 1150°F (upper bound), separator temperature = 95°F (lower bound), fresh toluene feed rate = 300 lb-mol/hr (upper bound), reactor inlet pressure = 500 psia (upper bound) and hydrogen to aromatic ratio in reactor inlet = 5 (lower bound) which based on self-optimizing control. They used a local (linear) analysis based on the SVD of the linearized model of the plant to select good candidate set for unconstrained controlled variables (Remaining degree of freedom). Unconstraint controlled variables are Mixer outlet methane mole fraction and Quencher outlet toluene mole fraction.

Chotirat Kiatpiriya (2007) followed the approach proposed by Skogestad (2000) based on Self-optimizing control and maximum scale gain for selected set of controlled variable. She studies only reaction section, first she control five active constraints follow by Antonio, Marius and Sigurd Skogestad (2006) and the remaining degree of freedom she used the maximum scale gain apply to select the best set of remaining controlled variables. She proposes different three control structures. Control structure one, methane mole fraction at the gas outlet separator with compressor power, reactor inlet temperature with furnace heat duty and percent toluene conversion at the plug flow reactor with the setpoint of the reactor temperature controller. Control structure two, methane mole fraction at the gas outlet separator with compressor power, reactor inlet temperature with furnace heat duty and benzene mole fraction at the separator bottom liquid outlet with the setpoint of the reactor temperature controller. Control structure three, methane mole fraction at the gas outlet separator with compressor power, reactor inlet temperature with furnace heat duty and reactor outlet temperature with the setpoint of the reactor temperature controller. She summary control structure three give better dynamic response and small loss when disturbance occur.

# CHAPTER III

# THEORY

## 3.1 Plantwide Control Structure Design Procedure

**Plantwide process control** involves the systems and strategies required to control an entire chemical plant consisting of many interconnected unit operations. A control engineers is typically presented a process flowsheet containing several recycles streams, energy integration and many different unit operation (distillation columns, heat-exchanger, reactor, etc.). Given such a complex, integrated process, one must devise the necessary logic, instrumentation and strategies to operate the plant safety and achieve its design objectives.

### 3.1.1 Basic concepts of plantwide control

Buckley (1964) was the first to suggest the idea of separating plantwide problem into two parts: material balance control and product quality control. He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loops is established, using flowrate of liquid and gas process streams. The idea is to establish the inventory control system by setting up this “hydraulic” control structure as the first step. Then he proposed establishing the product quality control loop by choosing appropriate manipulated variables.

Jim Douglas (1988) has devised a hierarchical approach to the conceptual design of process flowsheet. He points out that in the typical chemical plant the costs of raw materials and the value of products are usually much greater than the costs of capital and energy. This leads to the two Douglas doctrines:

1. Minimize losses of reactants and products.
2. Maximize flowrate though gas recycles systems.

The first idea implies that need tight control of stream composition exiting the process to avoid losses of reactants and products. The second rests on the principle that yield is worth more than energy.

Jim Downs (1992) pointed out the importance of looking at the chemical component balances around the entire plant and checking to see that the control structure handles these component balances effectively. He must ensure that all components (reactants, products and inert) have a way to leave or be consumed within the process.

Stephanopoulos et al. (1996) stated that the synthesis of a control system for a chemical plant. He asked: “Which variables should be measured in order to monitor completely the operation of a plant?” Which input should be manipulated for effective control? How measurements should be paired with the manipulations to form the control structure. He noted that the problem of plantwide control is “multi-objective” and there is a need for a systematic and organized approach which will identify all necessary control objectives. Their approaches respect the multi-objective nature of the design problem and take into account the propagation of disturbances in the process.

Luyben (1998) presented three laws have been developed as a result of number of case studies of many types of systems:

1. A stream somewhere in all recycle loops should be flow controlled. This is to prevent the snowball effect.
2. A fresh reactant feed stream cannot be flow controlled unless there is essentially complete one-pass conversion of one of the reactants. This law applies to systems with reaction types such as $A+B \rightarrow products$. In systems with consecutive reactions such as $A+B \rightarrow M+C$ and $M+B \rightarrow D+C$, the fresh fees can be flow controlled into the system because any imbalance in the ratios of reactants is accommodated by a shift in the amounts of the two products (M and D) that are generated. An excess of A will result in the production of more M and less D. An excess of B results in the production of more D and less M.
3. If the final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995). Changes in feed flowrate or feed composition have less of dynamic effect on distillate composition than they do on bottoms composition if the feed is saturated vapor: bottom is less affected than distillate. If our primary goal is to achieve tight product quality control, the basic column design should consider the dynamic implications of feed thermal conditions.

Bob Richardson suggested the heuristic that the largest stream should be selected to control the liquid level in a vessel it is called Richardson rule.

### 3.1.2 Steps of plantwide control structure design procedure

**Luyben et al. (1998)** presented **nine steps** of plantwide control design procedure satisfies the two fundamental chemical engineering principles, namely the overall conservation of energy and mass.

*Step 1: Establish control objectives*

Assess the steady-state design and dynamic control objectives for the process.

These objectives include reactor and separation yields, product quality specifications, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.

*Step 2: Determine control degrees of freedom*

Count the number of control valves available.

This is the number of degrees of freedom for control, i.e., the number of variables that can be controlled to setpoint. The valves must be legitimate (flow though a liquid-filled line can be regulated by only one control valve). The placement of these control valves can sometimes be made to improve dynamic performance, but often there is no choice in their location.

*Step 3: Establish energy management system*

Mask sure that energy disturbances do not propagate throughout the process by transferring the variability to the plant utility system.

They use the term energy management to describe two functions: (1) they must provide a control system that removes exothermic heats of reaction from the process. If heat is not removed to utilities directly at the reactor, then it can be used elsewhere in the process by other unit operations. (2) If heat integration does occur between process streams, then the second function of energy management is provide a control system that prevents the propagation of thermal disturbances and ensures the exothermic reactor heat is dissipated and not recycled.

*Step 4: Set production rate*

Establish the variables that dominate the productivity of the reactor and determine the most appropriate manipulator to control production rate.

Throughput changes can be achieved only by altering, either directly or indirectly, conditions in the reactor. To obtain higher production rates must increase overall reaction rates. For example, temperature is often a dominant reactor variable. If reactor temperature is not a dominant variable or cannot be changed for safety or yield reasons, in these cases you must find another dominant variable, such as the concentration of the limiting reactant, flowrate of initiator or catalyst to the reactor, reactor residence time, reactor pressure, or agitation rate.

*Step 5: Control product quality and handle safety, operational, and environmental constraints*

Select the "best" valves to control each of the product-quality, safety and environmental variables.

They want tight control of these important qualities for economic and operational reasons, Hence they should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants and deadtimes and large steady-state gains. It should be noted that establishing the product quality loops first, before the material balance control structure, is a fundamental difference between their plantwide control design procedure and Buckley's procedure.

*Step 6: Fix a flow in every recycle loop and control inventory (pressure and levels)*

Fix a flow in every recycle loop and then select the best manipulated variables to control inventories.

In most processes a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows that can occur if all flows in the recycle loop are controlled by levels. Gas recycle loops are normally set circulation rate, as limited by compressor capacity, to achieve maximum yields (Douglas doctrine). An inventory variable should typically be controlled with the manipulated variables that have the largest effect on it within that unit (Richardson rule).

*Step 7: Check component balances*

Identify how chemical components enter, leave, and generated or consumed in the process.

What are the methods or loops to ensure that the overall component balances for all chemical species are satisfied at steady-state? They don’t want reactant components to leave in the product streams because of the yield loss and the desired product purity specifications. Hence they are limited to the use of two methods: consuming the reactants by reaction or adjusting their fresh feed flow. Product and inert component all must have an exit path from the system. In many systems inert are moved by purging off a small fraction of the recycle stream. The purge rate is adjusted to control the inert composition in the recycle stream so that an economic balance is maintained between capital and operating costs.

*Step 8: Control individual unit operations*

Establish the control loops necessary to operate each of the individual unit operations.

Many effective control schemes have been established over the years for individual chemical units (Shinskey, 1988). For example, a tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flowrate to a furnace supplying energy to the reactor. Crystallizers require manipulation of refrigeration load to control temperature. Oxygen concentration in the stack gas from a furnace is controlled to prevent excess fuel usage. Liquid solvent feed flow to an absorber is controlled as some ratio to the gas feed.

*Step 9: Optimize economics or improve dynamic controllability*

Establish the best way to use the remaining control degree of freedom.

After satisfying all of the basic regulatory requirements, we usually have additional degrees of freedom involving control valves that have not been used and setpoints in some controllers that can be adjusted. These can be utilized either to optimize steady-state economic process performance (e.g., minimize energy, maximize selectivity) or to improve dynamic response.

**Truls Larsson and Skogestad (2000)** presented 8 steps of plantwide control design procedure. They combine step 1 and 9 of nine steps of Luyben (1998) for selection of controlled variables (control objectives) in step1. The procedure is divided in two main parts:

I: Top-down analysis (step 1-4), including definition of operational objectives and consideration of degree of freedom available to meet these.

II: Bottom-up design of the control system (step 5-8), starting with the stabilizing control layer.

Step 1: Definition of operational objectives.

Step 2: Manipulated variables and degrees of freedom.

Step 3: Primary controlled variables.

Step 4: Production rate.

Step 5: Regulatory control layer.

  5.1 Stabilization

  5.2 Local disturbance rejection

Step 6: Supervisory control layer.

  6a. Decentralized (single-loop) control

  6b. Multivariable control

Step 7: Optimization layer

Step 8: Validation

*Definition of operational objectives and constraints (step1)*

The operational objectives must be clearly defined before attempting to design a control system. Although this seems obvious, this step is frequently overlooked. Preferably, the operational objectives should be combined into a scalar cost function $J$ to be minimized. In many cases, $J$ may be simply selected as the operational cost, but there are many other possibilities. Other objectives, including safety constraints, should normally be formulated as constraints.

*Selection of manipulated variables and degree of freedom analysis (Step2)*

They start with the number of dynamic or control degrees of freedom, $N_m$ (m here denotes manipulated), which is equal to the number of manipulated variables. The number of manipulated variables *Nm* is usually easily obtained by process insight as the number of independent variables that can be manipulated by external means (typically, the number of adjustable valves plus other adjustable electrical and mechanical variables). Note that the original manipulated variables are always extensive variables.

Next, they identify the $N_{opt}$ optimization degrees of freedom, that is, the degrees of freedom that affect the operational cost $J$. In most cases, the cost depends on the steady-state only, and $N_{opt}$ equals the number of steady-state degrees of freedom $N_{ss}$. To obtain the number of steady-state degree of freedom they need to subtract from $N_m$:

- $N_{om}$ = The number of manipulated (input) variables with no steady-state effect (or more generally, with no effect on the cost). Typically, these are "extra" manipulated variables used to improve the dynamic response, e.g. an extra bypass on a heat exchanger.

- $N_{oy}$ = The number of (output) variables that need to be controlled, but which have no steady-state effect (or more generally, no effect on the cost). Typically, these are liquid levels in holdup tanks, and they have

$$N_{ss} = N_m - (N_{0m} + N_{0y})$$

The optimization is generally subject to constraints, and at the optimum many of these are usually "active". The number of "free" (unconstrained) degrees of freedom that are left to optimize the operation is then

$$N_{free} = N_{opt} - N_{active}$$

This is an important number, since it is generally for the unconstrained degrees of freedom that the selection of controlled variables.

*Self-optimizing control (steps 3)*

Self-optimizing control (Skogestad, 2000) is achieved if a constant setpoint policy results in an acceptable loss $L$ (without the need to reoptimize when disturbance occur). Their first control the variables directly related to ensuring optimal economic operation (these are the primary controlled variables $y_1 = c$ )

To select controlled variables for self-optimizing control, one may use the stepwise procedure of Skogestad (2000):

Step 3.1 Definition of optimal operation (cost and constraints)

Step 3.2 Determine degrees of freedom for optimization

Step 3.3 Identification of important disturbance

Step 3.4 Optimization (nominally and with disturbances)

Step 3.5 Identification of candidate controlled variables

Step 3.6 Evaluation of loss for alternative combinations of controlled variables (loss imposed by keeping constant setpoints when there are disturbances or implementation errors)

Step 3.7 Evaluation and selection (including controllability analysis)

To identify good candidate controlled variables, $c$ , one should look for variables that satisfy all of the following requirements :

- The optimal value of $c$ should be insensitive to disturbance.

- $c$ should be easy to measure and control (so that the implementation error is acceptable).
- The value of $c$ should be sensitive to changes in the manipulated variables (the steady-state degree of freedom). Equivalently, the optimum ($J$ as a function of $c$) should be flat.
- For case with more than one unconstrained degree of freedom, the selected controlled variables should be independent.

*Production rate and inventory control (step 4)*

The production rate is commonly assumed to be set at the inlet to plant, with outflows used for level control. They have the following rule: Identify the main bottleneck in the plant by optimizing the operation with the feedrate as a degree of freedom. Set the production rate at this location.

*Regulatory layer (step5)*

The main objective of regulatory control layer is to stabilize the plant. Usually it consists of single input-single output (SISO) PI control loops. The controlled variables for stabilization are measured output variables $y_2$, and their setpoint $y_2$ may be used as degree of freedom by the layers above.

A good secondary controlled variable (measurement) usually has the following properties:

- The variable is easy to measure
- The variable is easy to control using one of the available manipulated variables (the manipulated variable should have a "direct" fast and strong effect on it)
- For stabilization: The unstable mode should be detected "quickly" by the measurement (compute, for example, the pole vectors for a more detailed analysis)
- For local disturbance rejection: The variables is located "close" downstream of an important disturbance (use, for example, a partial control analysis for a more detailed analysis)

The "unstable" modes are very often related to inventory in each unit. This includes both the overall inventory (total mass) as well as the inventory of individual components.

- For liquid phase systems, overall inventory in each unit is stabilized by controlling liquid level.

- For gas phase systems, overall inventory (pressure) is controlled in selected units, but in many units it is left uncontrolled (floating), for example, to minimize pressure drop.
- For both gas and liquid phase systems, the inventory of individual components may need to be stabilized. Usually, this involves controlling a composition, or a derived property such as temperature. For example, in a distillation column, a temperature controller is often used to stabilize its otherwise drifting composition profile.

*Supervisory control (step6)*

They purpose the supervisor control layer is to keep the (primary) controlled outputs $c$ at their optimal setpoints $c_s$ , using degree of freedom the setpoints $y_{2s}$ in the regulatory layer and any unused manipulated inputs. For the supervisory control layer, the first structural issue is deciding on whether to used decentralized or multivariable control. Decentralized single-loop control is the simplest. It is preferred for non-interacting process and cases where active constraints remain constant. Multivariable control is preferred for interacting processes and for process with changes in active constraint.

*Optimization (step7)*

The purpose of the optimization is to identify the active constraints and recomputed optimal setpoints $c_s$ for controlled variables.

*Validation (step8)*

After having determined a plantwide control structure, it may be necessary to validate the structure, for example, using nonlinear dynamic simulation of critical parts.

## 3.2 New Plantwide Control Structure Design Procedure

Luyben et al. (1998) presented nine step of control structure design base on heuristic and engineering insight. Skogestad et al (2000) applied the nine steps by combination step 1 and 9 of Luyben for selection the controlled variables in step1. His purpose is receiving the best value of process operation for minimum utility.

This paper, we presented eight steps of control structure design base on heuristic combine with mathematics. The purpose of new plantwide control structure design is one easy way for selection the best set of control structure.

Normally, plantwide control design procedures consider decision about plant control structures in perspective. The plantwide control structure design is complex and confused. One easy way to deal with complexity is compartmentalizing it. However, the whole is greater than sum of its parts. There are properties (or behavior) of a system as whole emerge out of interaction of the components comprising the system. We must deal with both parts and system. The proposed plant design framework is shown in Figure 3.2 comprising of unit and plantwide level activities.

The general problems of control structure design are

1. Control objectives
2. Selection of controlled variables
3. Selection of manipulated variable
4. Selection of measurements
5. Selection of control configuration
6. Selection of controller type

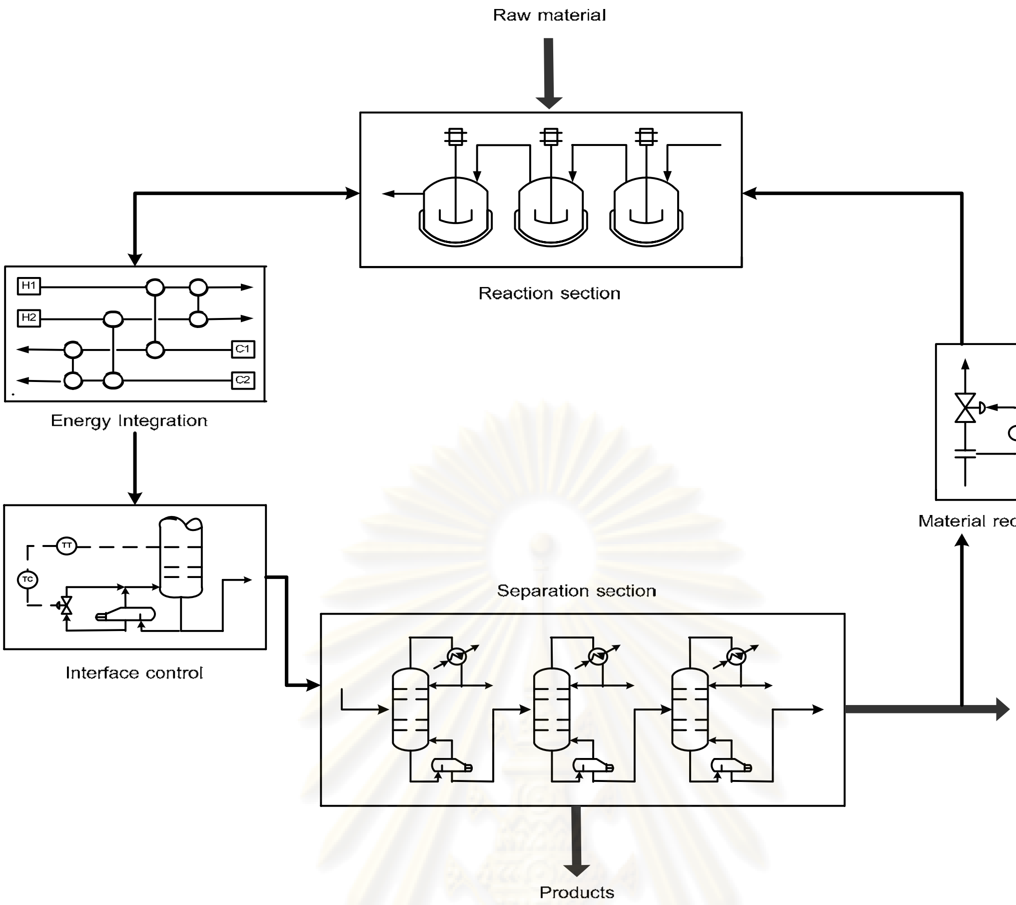


Figure 3.1 Flow diagram of the Plantwide control structure

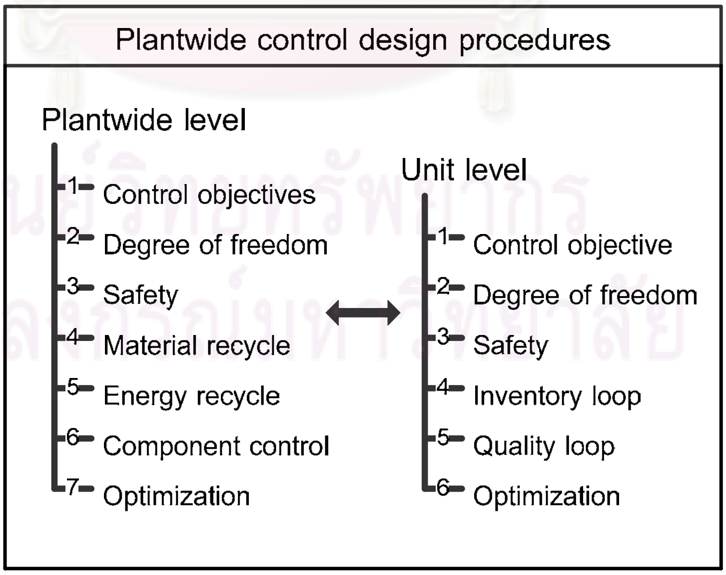


Figure 3.2 Typical of control hierarchy in plantwide control

### 3.2.1. Fixture point theorem

Hagglund (1995) present the real-time oscillation detection by calculates the integrated absolute deviation (IAE) between successive zero crossing of controller error signal. Its motivation is automatic monitoring of control-loop performance and detects oscillations in the control loop.

From his presented and the method of selection of controlled variable is proposed by Skogestad (2000), if we apply this idea of detection oscillations and sensitivity of process variables with disturbances for selection the controlled variable which can detect disturbances that propagate plantwide.

As mentioned above and the concept of material and energy disturbance propagation controls lead to fixture point theorem. Fixture point control theorem is transfixing point that given the most disturbance.

Fixture points theorem analysis

1. Identify key material variables (KMV) and key energy variables (KEV) from nature of process variables (large magnitude, high frequency and no quickly exit to surrounding).
2. Consideration at dynamic mode (open loop control) of Hysys simulation.
3. Steps of fixture point

Step1.Output (key process variables) screening technique: The candidate output (key process variables) can be considered by selecting the best in term of having the most disturbances from the selected inputs, i.e. having the largest IAE value. Change Input variables (MV and D) for ranking output sensitivity (The most sensitivity = key process variables)

Step2.Test load disturbance (Load disturbance = key process variables from step1) Rank the key process variables.

Step3.Normalize the IAE value which different units by maximum variation of each typical variable for bring it to summarize (Type of process variables are temperature, pressure, flowrate and composition)

Step4.Consider the first ranking of controlled variables: Considering key process variables that gives the most disturbance of other process variables (sum of normalize IAE value is large) should be controlled.

$$IAE = \int_0^\infty |e(t)|\,dt \tag{3.1}$$

As equation (3.1), $e(t) = \Delta y_i(t)$ is the change in i process variable on time t when key process j change (( $y_{K_j}$ ), when i and j=1, 2, 3 …n)

**Eight steps of our new control structure design procedure.**

The new plantwide control structure design procedure show as table 3.1.

**Table 3.1** A plantwide control structure design procedure.

| **Step of new plantwide control structure design.** |
|---|
| 1.Determine control objectives and operation constrains:<br>Identify control objectives (Plantwide and unit level)<br>Identify operational constraints |
| 2.Determine control degrees of freedom |
| 3.Handle safety operational and environmental constrains |
| 4.Set production rate |
| 5.Establish Key Control Structures:<br>Using fixture point theorem for mass pathway direction control |
| 6.Energy management |
| 7.Establish remaining individual unit operations |
| 8.Optimization via extra degrees of freedom |

*<u>Step1</u>. Determine control objectives and operation constrains*

Assess the steady-state design and dynamic control objective for the process. This is probably the most important aspect of the problem because different control objective leads to different control structures. The control objectives include satisfying the process constraints (including product quality). We identify the control objective by considering plantwide level and unit level.

<u>Plantwide level</u>: plantwide objectives should be formulated from the operation requirements of the plant. These control objectives typically include product quality and production rate.

<u>Unit level</u>: unit objective should be formulated from the stable operation of the plant. Perhaps, unit objective can used to minimize economic loss by applying self-

optimizing control. It relate to plantwide level. For example the distillation column, we can find the optimum condition (etc., the objective is purity of product) which minimize the loss of utility (Duty of condenser and reboiler operate at flat).

*Step2. Determine control degrees of freedom*

Traditionally, control degree of freedom is obtained by subtracting the sum of number of equations and externally defined variables from the number of variables. Luyben et al. proposed to count the number of control valves to find the control degree of freedom (DOF) of the process. This paper finds the DOF by Larsson (2000) method show in table 3.2.

**Table 3.2** Typical number of steady-state degree of freedom

| Process unit | DOF |
|---|---|
| Each external feed stream | 1 (feed rate) |
| Splitter | n-1 split fractions (n is the number of exit streams) |
| Mixer | 0 |
| Compressor, turbine, and pump | 1 (work) |
| Adiabatic flash tank | $0^a$ |
| Liquid phase reactor | 1 (holdup) |
| Gas phase reactor | $0^a$ |
| Heat exchanger | 1 (duty or net area) |
| Column (e.g. distillation) | |
| excluding heat exchangers | $0^a$ + number of side streams |

**Note:** a = Add 1 degree of freedom for each extra pressure that is set (need an extra valve, compressor, or pump), e.g., in flash tank, gas phase reactor, or column.

*Step3. Handle safety operational and environmental constrains*

Most chemical processes are inherently stable all operated at stable region. Although material recycle might cause system inoperable this come from snowball effect". Positive feedback all material recycle loop cause degradation in control performance.

By maintaining other control objective, i.e. loop that regulating material & energy flow in a process plant, some other objective are satisfy as the result for example safety and constraints regulation might be accomplish to higher control such as override control and selective control, emergency shutdown system (ESD)[WS].

Plantwide level: consider material recycle loop it causes a system to be born "snowball effect".

Unit level: the reactor is important unit for safety (temperature and pressure) condition.

*Step4. Set production rate*

This step involves identifying production rate manipulator selection. Decision the place where manipulation the production rate. Usually, from the main raw material to main product is used setting the production rate.

*Step5. Establish Keys Control Structure*

Plantwide system has the most interaction between unit operations, if we can detect the point that give the most sensitive with disturbances and big propagation to plantwide. Of course, this point should be control for disturbance rejection.

Step 1 to 4, we have set of process variables must be control for handle purity, production and safety operation. These variables came from engineering insight. This step, we use the fixture point analysis for indication the set of controlled variables for process stabilization.

First, screening output variables for identification to key process variables by using input variables change. The candidate output (key process variables) can be considered by selecting the best in term of having the most disturbances from the selected inputs, i.e. having the largest IAE value. After that, use the fixture point analysis for finding the rank of key process variables. We can pair the selected key process variable with manipulated variable follow by order ranking.

Rules for selecting manipulated variable (MV) to control key process variable (KPV)

1. Select manipulated variable that is good controllability for key process variable.
2. Select manipulated variable to maximize the magnitude of the (scale) gain from MV to KPV.
3. Avoid the manipulated variables that may saturate.

*Step6. Energy management*

To avoid heat removals from the thermal sinks and prevent propagation of thermal disturbance. We use the term energy management to describe two functions.

4. We must provide a control system that removes exothermic heats of reaction from the process. If heat of reaction is not removed to utilities directly then it can propagate to plantwide and effect to other units operation.
5. If heat integration does occur between process streams, then the second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensure the exothermic reactor heat is dissipated and not recycled. Process-to-process heat exchanger and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

*Step7. Establish remaining individual unit operation*

Control of individual unit operation is considered priority to checking component material balances. This step taken care composition loops (or temperature loops) and other loops (levels and pressures) of all the individual unit operations.

1. For liquid phase systems, overall inventory in each unit is stabilized by controlling liquid level.
2. For gas phase systems, controlling pressure for prevention floating condition.
3. For compositions, we do not need to control the inventory of all components but should consider single component that effect to several components. Usually, the composition controlling in distillation column related to temperature so used it to stabilize the composition profile.

*Step8. Optimization via extra degree of freedom*

Many a times, the job of control engineer is placement the control valves in the process flow diagram which needs the improving dynamic controllability and reduce economic loss. The extra degree of freedom in this step includes the remaining degree of freedom.

## 3.3 Steady-State Gain

The availability of accurate steady-state gains for a multivariable process facilitates significantly the control system design procedure. The steady-state gains provide the zero frequency characteristics of the system. This piece of information enables the initial screening and selection of proper manipulated and/ or controlled variables, variable pairing, and initial evaluation of candidate control structures (Grosdidier et al., 1985: Yu and Luyben, 1986; Shinskey, 1988).

The steady-state gains can be determined by using either plant tests (although it has been shown (Luyben, 1987a) that the results might be seriously different from those of a linearized model of the process) or some kind of a rating program (Buckley et al., 1985). A third and more complex alternative is to get the steady-state gains through a transfer function identification procedure, if dynamic plant data or data from a dynamic model of the process are available.

The usual method to determine the gains is an open loop type of test. A specific control structure is assumed. A small perturbation is introduced in one of the manipulated variables. All the remaining manipulated variables are held constant. The rating program is converged. All measurement variables changes are recorded. The steady-state gain between the *i* controlled variable and the *j* manipulated variable is calculated as

$$g_{ij} = \Delta x_{ij} / \Delta m_j \quad i = 1,2,...,n;\ j = 1,2,...,m \tag{3.2}$$

where $g$ , is the *ij* element of the gain matrix and $\Delta x_{ij}$ is the change in the *i* controlled variable because of the $\Delta m_j$ change in the *j* manipulated variable.

According to this procedure, *m* tests need to be performed for every candidate control structure where m is the number of manipulated variables. For controlled variable selection, this procedure is ideal because it provides gains for all controlled variables.

The problem of the effect of scaling on the steady-state gains process is handled by expressing the gains of all the plant transfer functions in dimensionless form. The gains with engineering units are divided by transmitter spans and multiplied by valve gains. The method for scaling on the steady-state gains are elucidated below.

## 3.4 Scaling

Scaling is very important in practical applications as it makes model analysis and controller design (weight selection) much simpler. It requires the engineer to make a judgment at the start of the design process about the required performance of the system. To do this, decisions are made on the expected magnitudes of disturbance and reference changes, on the allowed magnitude of each input signal, and on the allowed deviation of each input. Let the unscaled (or originally scaled) linear model of the process in deviation variable be

$$\hat{y} = \hat{G}\hat{u} + \hat{G}_d \hat{d}; \quad \hat{e} = \hat{y} - \hat{r} \tag{3.3}$$

Where a hat (^) is used to show that the variables are in their unscaled units. A useful approach for scaling is to make the variables less than 1 in magnitude. This is done by dividing each variable by its maximum expected or allowed change. For disturbances and manipulated inputs, we used the scaled variables

$$d = \hat{d} / \hat{d}_{\max}, \quad u = \hat{u} / \hat{u}_{\max} \tag{3.4}$$

where:

- $\hat{d}_{\max}$ - largest expected change in disturbance
- $\hat{u}_{\max}$ - largest allowed input change

The maximum deviation from a nominal value should be chosen by thinking of the maximum value one can expect, or allow, as function of time. The variables $\hat{y}, \hat{e}$ and $\hat{r}$ are in the same units, so the same scaling factor should be applied to each. Two alternatives are possible:

- $\hat{e}_{\max}$ - largest allowed control error
- $\hat{r}_{\max}$ - largest expected change in reference value

Since a major objective of control is to minimize the control error, we here usually choose to scaled with respect to the minimum control error:

$$y = \hat{y} / \hat{e}_{\max}, \ \ r = \hat{r} / \hat{e}_{\max}, \ \ e = \hat{e} / \hat{e}_{\max} \tag{3.5}$$

# CHAPTER IV

# PROCESS DESCRIPTION AND CASE STUDY

## 4.1 HDA process description for case study

In the HDA process, fresh toluene (pure) and hydrogen (97% hydrogen and 3% methane) are mixed with the recycled toluene and hydrogen (Figure 4.1A).

This reactant mixture is preheated in a feed-effluent heat exchanger (FEHE) using the reactor effluent stream and then to the reaction temperature in a furnace before being fed to adiabatic plug flow reactor (PFR). Two main reaction taking place inside this reactor are

$$Toluene + H_2 \rightarrow Benzene + Methane \tag{4.1}$$

$$2Benzene \leftrightarrow Diphenyl + H_2 \tag{4.2}$$

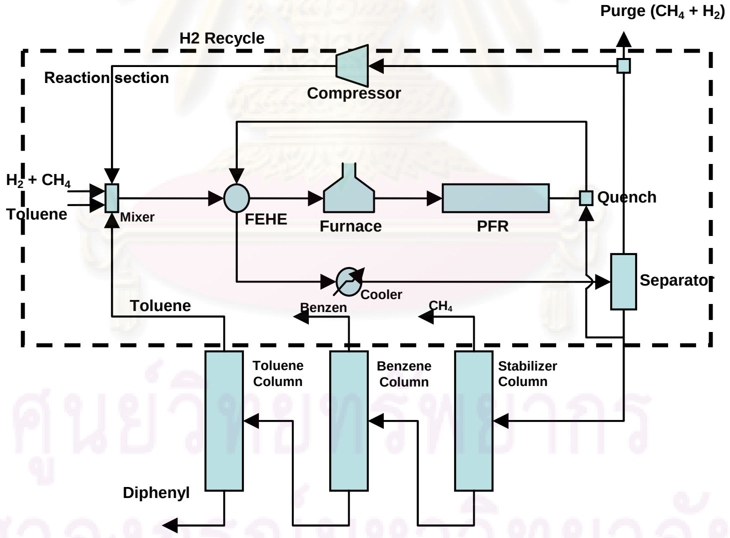


Figure 4.1A The Hydrodealkylation process (Luyben 1998)

The kinetic rate expressions are functions of the partial pressure (psia unit) of toluene $p_T$, hydrogen $p_H$, benzene $p_B$, and diphenyl $p_D$ with an Arrhenius temperature dependence. Zimmerman and York (1964) provide the following rate expression

$$\begin{aligned} r_1 &= 3.6858\times10^6 \exp(-25616/T)P_T P_B^{1/2} \\ r_2 &= 5.987\times10^4 \exp(-25616/T)P_B^2 - 2.553\times10^5 \exp(-25616/T)P_D P_H \end{aligned} \tag{4.3}$$

Where $r_1$ and $r_2$ have units of $lbmol/(\min \times ft^3)$ and T is the absolute temperature in Kelvin. The heats of reaction given by Douglas (1988) are -21500 Btu/lbmol of toluene for $r_1$ and 0 Btu/lbmol for $r_2$

The reactor effluent is quenched with a portion of the recycle separator liquid to prevent coking and further cooled in the FEHE and cooler before being fed to the flash separator. A portion of the unconverted hydrogen and methane overhead vapor from the separator is purged (to avoid accumulation of methane within the process) while the remainder in compressed and recycled to the reactor. The liquid from the separator is processed in the separation section consisting of three distillation columns. The stabilizer column removes hydrogen and methane as the overhead product, and benzene is the desired product from the benzene column top. Finally, in the toluene column, toluene is separated from diphenyl, as the distillate and recycled back to the process.

### 4.1.1 Steady-state modeling

The model of the HDA process used in this paper is a version of the model developed by Luyben (2002).A flowsheet of the Hysys model show in Figure 4.1B. The flowsheet streams data taken from Antonio, Marius and Sigurd Skogestad (2006) show in table 5. The equipment designs follow from Douglas (1988) and Luyben et al. (1998).

The Peng-Robinson (PR) equation of state is selected for the property estimation as it is very reliable for predicting the properties of hydrocarbons over a wide range of conditions and is generally recommended for oil, gas and petrochemical applications.

### 4.1.2 Operation constraints

1. Minimum production rate

   D benzene $\geq$ 265 lbmol/h

2. Hydrogen to aromatic ratio in reactor inlet (Prevent coking)

   rH2 $\geq$ 5

3. Maximum toluene feed rate

   F toluene $\leq$ 300 lbmol/h

4. Reactor inlet pressure

   P reactor $\leq$ 500 psia

5. Reactor outlet temperature (Prevent hydro cracking reaction)

   T reactor, out $\leq$ 1300 F

6. Quencher outlet temperature

(Prevent thermal decomposition of products and to avoid fouling in FEHE)

$T_{\text{quencher, out}} \leq 1150$ F

7. Product purity at the benzene column distillation

$X_{D,\text{ benzene}} \geq 0.9997$

8. Separator inlet temperature

95 F $\leq T_{\text{separator, in}} \leq$ 105 F

9. Reactor inlet temperature: To get high enough reactor rates

(Luyben (1998), Sigurd Skogestad and Antonio, (2006))

**Table 4.1** Equipment data of reaction section

| Unit | | Specification |
|---|---|---|
| RX (Reactor): | | |
| | Diameter (ft) | 9.53 |
| | Length (ft) | 57 |
| | Number of tube | 1 |
| HX (Heat-Exchanger): | | |
| | Shell volume ($ft^3$) | 500 |
| | Tube volume ($ft^3$) | 500 |
| FUR (Furnace): | | |
| | Volume ($ft^3$) | 300 |
| COND (Condenser): | | |
| | Volume ($ft^3$) | 300 |
| SEP (Separator): | | |
| | Volume ($ft^3$) | 80 |

**Table 4.2** Equipment data of separation section

| Unit | | Specification |
|---|---|---|
| Stabilizer column: | | |
| | Number of theoretical trays | 6 |
| | Feed tray | 3 |
| | Diameter (ft) | 1 |
| | Reboiler volume ($ft^3$) | 250 |
| | Condenser volume ($ft^3$) | 7.5 |
| Benzene column: | | |
| | Number of theoretical trays | 27 |
| | Feed tray | 15 |
| | Diameter (ft) | 5.7 |
| | Reboiler volume ($ft^3$) | 316 |
| | Condenser volume ($ft^3$) | 293 |
| Toluene column: | | |
| | Number of theoretical trays | 7 |
| | Feed tray | 5 |
| | Diameter (ft) | 2.5 |
| | Reboiler volume ($ft^3$) | 46 |
| | Condenser volume ($ft^3$) | 36 |

### 4.1.3 Degree of freedom analysis

**Table 4.3** Typical number of steady-state degree of freedom for some process units

| Process unit | DOF |
|---|---|
| Each external feed stream | 1 (feed rate) |
| Splitter | n-1 split fractions (n is the number of exit streams) |
| Mixer | 0 |
| Compressor, turbine, and pump | 1 (work) |
| Adiabatic flash tank | $0^a$ |
| Liquid phase reactor | 1 (holdup) |
| Gas phase reactor | $0^a$ |
| Heat exchanger | 1 (duty or net area) |
| Column (e.g. distillation) excluding heat exchangers | $0^a$ + number of side streams |

**Note** a = Add 1 degree of freedom for each extra pressure that is set (need an extra valve, compressor, or pump), e.g., in flash tank, gas phase reactor, or column.

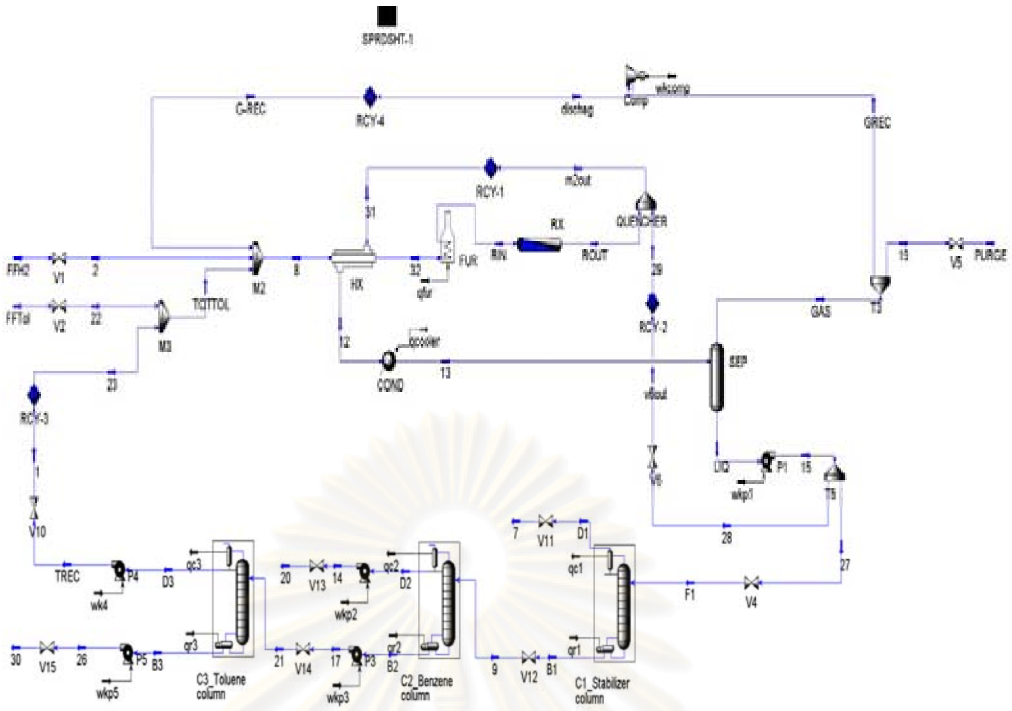


**Figure 4.1B** Hydrodealkylation (HDA) Hysys process flow sheet.

### 4.1.4 Manipulated variables

| Number | symbol | List of overall manipulabel variables |
|---|---|---|
| 1 | V1 | Hydrogen fresh feed valve |
| 2 | V2 | Toluene fresh feed valve |
| 3 | V4 | Stabilizer feed valve |
| 4 | V5 | Purge gas valve |
| 5 | V6 | Flow of cooling stream to quencher valve |
| 6 | Qfur | Furnace heat duty |
| 7 | Qcooler | Cooler heat duty |
| 8 | Wkcomp | Compressor power |
| 9 | V10 | Toluene recycle valve |
| 10 | V11 | Stabilizer column overhead valve |
| 11 | V12 | Stabilizer column bottom valve |
| 12 | V13 | Benzene column overhead valve |
| 13 | V14 | Benzene column bottom valve |
| 14 | V15 | Toluene column bottom valve |
| 15 | qc1 | Stabilizer column condenser heat duty |
| 16 | qc2 | Benzene column condenser heat duty |
| 17 | qc3 | Toluene column condenser heat duty |
| 18 | qr1 | Stabilizer column reboiler heat duty |
| 19 | qr2 | Benzene column reboiler heat duty |
| 20 | qr3 | Toluene column reboiler heat duty |

Table 4.4 Stream table for the nominally optimal operating point for the HDA process

| Name | FFH2 | FFTol | 2 | 22 | 8 | TOTTOL | 32 | 31 | 12 | RIN | ROUT | 13 | GAS | LIQ | GREC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| vapor fraction | 1.0000 | 0.0000 | 1.0000 | 0.0000 | 0.9298 | 0.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 0.9024 | 1.0000 | 0.0000 | 1.0000 |
| temperature (F) | 100.00 | 100.00 | 100.00 | 100.33 | 120.92 | 116.85 | 1004.79 | 1150.37 | 361.12 | 1201.20 | 1270.68 | 95.00 | 95.00 | 95.00 | 95.00 |
| pressure (psia) | 605.00 | 605.00 | 555.00 | 555.00 | 555.00 | 555.00 | 535.00 | 496.00 | 477.40 | 500.00 | 496.00 | 477.00 | 477.00 | 477.00 | 477.00 |
| total flow (lbmole/h) | 446.77 | 300.00 | 446.77 | 300.00 | 5063.49 | 325.98 | 5063.49 | 5246.55 | 5246.55 | 5063.49 | 5063.50 | 5246.55 | 4734.31 | 512.24 | 4331.89 |
| mole fraction | | | | | | | | | | | | | | | |
| hydrogen | 0.9700 | 0.0000 | 0.9700 | 0.0000 | 0.3591 | 0.0000 | 0.3591 | 0.2918 | 0.2918 | 0.3591 | 0.3022 | 0.2918 | 0.3230 | 0.0034 | 0.3230 |
| methane | 0.0300 | 0.0000 | 0.0300 | 0.0000 | 0.5691 | 0.0000 | 0.5691 | 0.6081 | 0.6081 | 0.5691 | 0.6283 | 0.6081 | 0.6682 | 0.0522 | 0.6682 |
| benzene | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0072 | 0.0001 | 0.0072 | 0.0887 | 0.0887 | 0.0072 | 0.0619 | 0.0887 | 0.0084 | 0.8308 | 0.0084 |
| toluene | 0.0000 | 1.0000 | 0.0000 | 1.0000 | 0.0646 | 0.9998 | 0.0646 | 0.0080 | 0.0080 | 0.0646 | 0.0054 | 0.0080 | 0.0003 | 0.0792 | 0.0003 |
| diphenyl | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0034 | 0.0034 | 0.0000 | 0.0022 | 0.0034 | 0.0000 | 0.0344 | 0.0000 |
| molar flow (lbmole/h) | | | | | | | | | | | | | | | |
| hydrogen | 433.37 | 0.00 | 433.37 | 0.00 | 1818.41 | 0.00 | 1818.41 | 1531.09 | 1531.09 | 1818.41 | 1530.14 | 1531.09 | 1529.34 | 1.75 | 1399.34 |
| methane | 13.40 | 0.00 | 13.40 | 0.00 | 2881.61 | 0.00 | 2881.61 | 3190.37 | 3190.37 | 2881.61 | 3181.16 | 3190.37 | 3163.65 | 26.72 | 2894.74 |
| benzene | 0.00 | 0.00 | 0.00 | 0.00 | 36.33 | 0.05 | 36.33 | 465.51 | 465.51 | 36.33 | 313.32 | 465.51 | 39.93 | 425.58 | 36.54 |
| toluene | 0.00 | 300.00 | 0.00 | 300.00 | 327.13 | 325.92 | 327.13 | 41.96 | 41.96 | 327.13 | 27.59 | 41.96 | 1.38 | 40.57 | 1.27 |
| diphenyl | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 | 17.62 | 17.62 | 0.01 | 11.29 | 17.62 | 0.00 | 17.61 | 0.00 |

Table 4.4 (Continued) Stream table for the nominally optimal operating point for the HDA process

| Name | 19 | PURGE | 15 | 28 | 27 | 29 | m2out | v6out | F1 | D1 | B1 | 9 | G-REC | B2 | D2 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| vapor fraction | 1.0000 | 1.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0000 | 0.0000 | 0.0340 | 1.0000 | 0.0000 | 0.4500 | 1.0000 | 0.0000 | 0.0000 |
| temperature (F) | 95.00 | 93.47 | 95.31 | 95.31 | 95.31 | 95.51 | 1150.45 | 95.51 | 96.15 | -70.10 | 366.79 | 233.96 | 122.74 | 312.34 | 221.99 |
| pressure (psia) | 477.00 | 427.00 | 530.00 | 530.00 | 530.00 | 496.00 | 496.00 | 496.00 | 150.31 | 150.00 | 150.51 | 31.00 | 555.00 | 32.16 | 30.00 |
| total flow (lbmole/h) | 402.42 | 402.42 | 512.24 | 183.89 | 328.35 | 183.39 | 5246.89 | 183.89 | 328.35 | 18.25 | 310.09 | 310.09 | 4290.74 | 37.26 | 272.83 |
| mole fraction | | | | | | | | | | | | | | | |
| hydrogen | 0.3230 | 0.3230 | 0.0034 | 0.0034 | 0.0034 | 0.0034 | 0.2917 | 0.0034 | 0.0034 | 0.0615 | 0.0000 | 0.0000 | 0.3228 | 0.0000 | 0.0000 |
| methane | 0.6682 | 0.6682 | 0.0522 | 0.0522 | 0.0522 | 0.0521 | 0.6081 | 0.0522 | 0.0522 | 0.9384 | 1.00E-06 | 0.0000 | 0.6685 | 0.0000 | 0.0000 |
| benzene | 0.0084 | 0.0084 | 0.8308 | 0.8308 | 0.8308 | 0.8314 | 0.0888 | 0.8308 | 0.8308 | 0.0001 | 0.8797 | 0.8797 | 0.0085 | 0.0013 | 0.9997 |
| toluene | 0.0003 | 0.0003 | 0.0792 | 0.0792 | 0.0792 | 0.0784 | 0.0080 | 0.0792 | 0.0792 | 0.0000 | 0.0839 | 0.0839 | 0.0003 | 0.6957 | 0.0003 |
| diphenyl | 0.0000 | 0.0000 | 0.0344 | 0.0344 | 0.0344 | 0.0346 | 0.0034 | 0.0344 | 0.0344 | 0.0000 | 0.0364 | 0.0364 | 0.0000 | 0.3030 | 0.0000 |
| molar flow (lbmole/h) | | | | | | | | | | | | | | | |
| hydrogen | 129.99 | 129.99 | 1.75 | 0.63 | 1.12 | 0.63 | 1530.77 | 0.63 | 1.12 | 1.12 | 0.00 | 0.00 | 1385.04 | 0.00 | 0.00 |
| methane | 268.91 | 268.91 | 26.72 | 9.59 | 17.13 | 9.56 | 3190.72 | 9.59 | 17.13 | 17.13 | 0.00 | 0.00 | 2868.20 | 0.00 | 0.00 |
| benzene | 3.39 | 3.39 | 425.58 | 152.78 | 272.80 | 152.48 | 465.80 | 152.78 | 272.80 | 0.00 | 272.80 | 272.80 | 36.28 | 0.05 | 272.75 |
| toluene | 0.12 | 0.12 | 40.57 | 14.57 | 26.01 | 14.37 | 41.96 | 14.57 | 26.01 | 0.00 | 26.01 | 26.01 | 1.21 | 25.93 | 0.08 |
| diphenyl | 0.00 | 0.00 | 17.61 | 6.32 | 11.29 | 6.35 | 17.64 | 6.32 | 11.29 | 0.00 | 11.29 | 11.29 | 0.00 | 11.29 | 0.00 |

Table 4.4 (Continued) Stream table for the nominally optimal operating point for the HDA process

| Name | 23 | 17 | 14 | 20 | 7 | 21 | B3 | D3 | 26 | 30 | TREC | 1 | dischag |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| vapor fraction | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0000 | 0.0236 | 0.0000 | 0.0000 | 0.0000 | 0.0019 | 0.0000 | 0.0000 | 1.0000 |
| temperature (F) | 285.01 | 312.61 | 222.39 | 222.49 | -80.09 | 307.84 | 557.10 | 279.68 | 557.35 | 557.11 | 284.62 | 285.01 | 122.74 |
| pressure (psia) | 555.00 | 82.16 | 80.00 | 50.00 | 50.00 | 30.17 | 30.50 | 30.00 | 80.50 | 30.50 | 675.00 | 555.00 | 555.00 |
| total flow (lbmole/h) | 25.98 | 37.26 | 272.83 | 272.83 | 18.25 | 37.26 | 11.28 | 25.98 | 11.28 | 11.28 | 25.98 | 25.98 | 4331.89 |
| mole fraction | | | | | | | | | | | | | |
| hydrogen | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0615 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.3230 |
| methane | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.9384 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.6682 |
| benzene | 0.0019 | 0.0013 | 0.9997 | 0.9997 | 0.0001 | 0.0013 | 0.0000 | 0.0019 | 0.0000 | 0.0000 | 0.0019 | 0.0019 | 0.0084 |
| toluene | 0.9976 | 0.6957 | 0.0003 | 0.0003 | 0.0000 | 0.6957 | 0.0004 | 0.9976 | 0.0004 | 0.0004 | 0.9976 | 0.9976 | 0.0003 |
| diphenyl | 0.0005 | 0.3030 | 0.0000 | 0.0000 | 0.0000 | 0.3030 | 0.9996 | 0.0005 | 0.9996 | 0.9996 | 0.0005 | 0.0005 | 0.0000 |
| molar flow (lbmole/h) | | | | | | | | | | | | | |
| hydrogen | 0.00 | 0.00 | 0.00 | 0.00 | 1.12 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1399.34 |
| methane | 0.00 | 0.00 | 0.00 | 0.00 | 17.13 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 2894.74 |
| benzene | 0.05 | 0.05 | 272.75 | 272.75 | 0.00 | 0.05 | 0.00 | 0.05 | 0.00 | 0.00 | 0.05 | 0.05 | 36.54 |
| toluene | 25.92 | 25.93 | 0.08 | 0.08 | 0.00 | 25.93 | 0.00 | 25.92 | 0.00 | 0.00 | 25.92 | 25.92 | 1.27 |
| diphenyl | 0.01 | 11.29 | 0.00 | 0.00 | 0.00 | 11.29 | 11.28 | 0.01 | 11.28 | 11.28 | 0.01 | 0.01 | 0.00 |

| Name | qfur | qcooler | wkcomp | qr1 | qc1 | qr2 | qc2 | qr3 | qc3 |
|---|---|---|---|---|---|---|---|---|---|
| Btu/h | 1.57E+07 | 2.17E+07 | 9.57E+05 | 9.82E+03 | 3.78E+06 | 8.53E+06 | 1.02E+07 | 7.00E+05 | 4.19E+05 |

## 4.2 New plantwide control structure design procedure

**Table 4.5** Improved heuristic methodology

| Step of new plantwide control structure design. |
|---|
| 1.Determine control objectives and operation constrains:<br>Identify control objectives (Plantwide and unit level)<br>Identify operational constraints |
| 2.Determine control degrees of freedom |
| 3.Handle safety operational and environmental constrains |
| 4.Set production rate |
| 5.Establish Key Control Structures:<br>Using fixture point theorem for mass pathway direction control |
| 6.Energy management |
| 7.Establish remaining individual unit operations |
| 8.Optimization via extra degrees of freedom |

## 4.3 Case Study

This section describes the fixture point control procedure applied to the HDA process model in Hysys starting with the control objectives.

### 4.3.1 Plantwide Control Strategy

Step 1 Determine control objectives and operation constrains

The objectives we decomposed into two levels: Plantwide level and Unit level. Plantwide objectives typically include production rate, product quality and minimum economic loss. Unit operation objectives typically include equipment constrains, safety concern and smooth operation (process stability).

*HDA process:*

Plantwide objectives:

The goals of plantwide are to produce benzene product at 265 lbmole/hr with 0.9997 purity and minimum loss of economic. We use the optimum value operation follow by Araujo et al. (2006) for minimum utility usage in normal operating point.

Unit operation objectives:

The goals of unit operation are avoid drift of process variables (process stability) and control equipment constrains.

Summary:

(1) Production rate: 265 lbmole/hr

(2) Product quality: benzene purity ≥ 99.97 %

(3) Following by Araujo et al, 2006 specify 6 variables for distillation column to minimize economic loss.

(4) Process constrains:

1. The reactor inlet temperature should be around 1150$^{o}$F. This is an optimization decision to have better reaction rate.

2. The reactor outlet temperature should not exceed 1300$^{o}$F to avoid coking.

3. The outlet stream from the reactor must be quenched to 1150$^{o}$F to prevent thermal decomposition of products and avoid fouling in heat-exchanger.

4. The ratio of hydrogen to aromatics (benzene, toluene and diphenyl) has to be at least five at the reactor inlet. Excess hydrogen encourages the primary reaction and discourages the secondary reaction.

Step 2 Determine control degrees of freedom

From table 4.6 we have 13 steady-state degrees of freedom and 7 liquid levels that need to be controlled which have no steady-state effect. So we have 20 manipulated variables for control structure design.

**Table 4.6** Steady-state degree of freedom analysis (Skogestad, 2002)

| Process unit | DOF |
|---|---|
| Each external feed stream | 2 x 1 = 2 |
| Splitter (purge and quench) | 2 x 1 = 2 |
| Compressor | 1 x 1 = 1 |
| Adiabatic flash tank (separator) | 1 x 0 = 0 |
| Gas phase reactor | 1 x 0 = 0 |
| Heat exchanger in reaction section (furnace and cooler) | 2 x 1 = 2 |
| Heat exchanger in distillation section (3 distillation column) | 3 x 2 = 6 |
| Total | 13 |

Step 3 Handle safety operational and environmental constrains

Plantwide level:

Consider material recycle loop it causes a system to be born “snowball effect”. HDA processes have two recycle streams: gas recycle and liquid recycle, we focus on gas recycle because liquid recycle is pure toluene reactant (a little contaminates) but gas recycle have more methane contaminate lead to snowball effect. Therefore one method use for avoid snowball effect is control the methane composition in the process.

Unit level:

The reactor is important unit because it has gas phase exothermic reaction (unstable unit operation). The reactor can operate at maximum temperature of catalyst damaging or result in a vessel meltdown. The temperature and pressure of reactor should be controlled.

Step 4 Set production rate

Three positions used for set production rate: one reactor inlet temperature to get high enough reaction rates, two quantities of toluene reactant (limiting reactant) feed into reactor and three hydrogen feed streams because steady-state simulation tell us the side reaction occur about 60% conversion of benzene product so the hydrogen is good sensitivity for limit side reaction. (Usually, the reactor inlet temperature is fixed for safety and side reaction control by quencher temperature indirectly, so one way for set production rate is fixing fresh feed toluene.)

Step 5 Establish Keys Control Structure

All processes have the key points (type and placement of process variables) meaning if the disturbance occurs in the process, the key points are most varied. In a similar way if we know what variable most affect to other variables, we can control the direction of it (key variables) for control disturbance propagation in the process.

Because the toluene conversion in the reactor is high ($\approx 95\%$), the result is that the liquid recycle (toluene recycle) is small. Therefore, we separate into reaction section and separation section of the control structure designs. In the reaction section we select key control variables from fixture point theorem and in the separation section we select control variable from sensitivity method.

*Output (key process variables) screening*

First, screening output variables for identification key process variables by using input variables change (change one percent of manipulated variables and disturbance variables (temperature, pressure and flow rate of fresh feed streams)).The result shown as below (reaction section only).

**Table 4.7** Key process variables screening

| Temperature variable | | |
|---|---|---|
| position | Symbol of position on flowsheet | IAE value |
| Reactor inlet stream | RIN | 8.54 |
| Reactor out stream | ROUT | 8.25 |
| Quencher outlet stream | m2out | 8.13 |
| Gas recycle stream | G-REC | 7.30 |
| Separator inlet stream | 13 | 7.25 |
| Separator liquid stream | LIQ | 7.22 |
| Separator vapor stream | GAS | 7.22 |
| Compressor inlet stream | GREC | 7.22 |
| Purge stream | PURGE | 7.16 |
| Liquid stream to stabilizer column | F1 | 7.12 |
| Mixture stream | 8 | 5.57 |
| Pressure variable | | |
| position | Symbol of position on flowsheet | IAE value |
| Separator inlet stream | 13 | 1.72 |
| Separator vapor stream | GAS | 1.72 |
| Separator liquid stream | LIQ | 1.72 |
| Compressor inlet stream | GREC | 1.72 |
| Reactor outlet stream | ROUT | 1.66 |
| Quencher outlet stream | m2out | 1.66 |
| Reactor inlet stream | RIN | 1.64 |
| Mixture stream | 8 | 1.57 |
| Total toluene stream | TOTTOL | 1.57 |
| Gas recycle stream | G-REC | 1.57 |

Table 4.7 (Continue) Key process variables screening

| Flow variable | | |
|---|---|---|
| position | Symbol of position on flowsheet | IAE value |
| Quencher outlet stream | m2out | 72.63 |
| Separator inlet stream | 13 | 72.52 |
| Mixture stream | 8 | 70.77 |
| Reactor inlet stream | RIN | 70.74 |
| Reactor outlet stream | ROUT | 70.67 |
| Separator vapor stream | GAS | 67.83 |
| Compressor inlet stream | GREC | 64.30 |
| Gas recycle stream | G-REC | 64.30 |
| Methane composition variable | | |
| position | Symbol of position on flowsheet | IAE value |
| Separator vapor stream | GAS | 0.0185 |
| Compressor inlet stream | GREC | 0.0185 |
| Gas recycle stream | G-REC | 0.0185 |
| Purge stream | PURGE | 0.0185 |
| Reactor outlet stream | ROUT | 0.0172 |
| Quencher outlet stream | m2out | 0.0166 |
| Mixture stream | 8 | 0.0152 |
| Reactor inlet stream | RIN | 0.0152 |
| Hydrogen composition variable | | |
| position | Symbol of position on flowsheet | IAE value |
| Separator vapor stream | GAS | 0.0199 |
| Compressor inlet stream | GREC | 0.0199 |
| Gas recycle stream | G-REC | 0.0199 |
| Purge stream | PURGE | 0.0199 |
| Reactor outlet stream | ROUT | 0.0188 |
| Quencher outlet stream | m2out | 0.0182 |
| Mixture stream | 8 | 0.0173 |
| Reactor inlet stream | RIN | 0.0173 |
| Benzene composition variable | | |
| position | Symbol of position on flowsheet | IAE value |
| Separator liquid stream | LIQ | 0.0179 |
| Liquid stream to stabilizer column | F1 | 0.0179 |
| Quencher outlet stream | m2out | 0.0027 |
| Reactor outlet stream | ROUT | 0.0023 |

**Table 4.7** (Continue) Key process variables screening

| Toluene composition variable | | |
|---|---|---|
| position | Symbol of position on flowsheet | IAE value |
| Liquid stream to stabilizer column | F1 | 0.0238 |
| Separator liquid stream | LIQ | 0.0238 |
| Quencher outlet stream | m2out | 0.0024 |
| Reactor outlet stream | ROUT | 0.0017 |
| Biphenyl composition variable | | |
| position | Symbol of position on flowsheet | IAE value |
| Liquid stream to stabilizer column | F1 | 0.0072 |
| Separator liquid stream | LIQ | 0.0072 |
| Quencher outlet stream | m2out | 0.0007 |
| Reactor outlet stream | ROUT | 0.0005 |
| position | parameter | IAE value |
| Reactor inlet stream | Hydrogen to aromatic ratio | 0.3907 |
| PFR | Toluene conversion | 0.0260 |

**Table 4.8** Ranks of key process variables from fixture point analysis. (Reaction section)

| Rank | Key process variables | Sum IAE |
|---|---|---|
| 1 | Quencher outlet temperature | 22.81 |
| 2 | Reactor inlet temperature | 21.49 |
| 3 | Reactor outlet temperature | 21.03 |
| 4 | Separator pressure | 16.96 |
| 5 | Compressor inlet pressure | 13.96 |
| 6 | Compressor outlet pressure | 13.30 |
| 7 | Mixer outlet temperature | 10.53 |
| 8 | Mixer outlet pressure | 8.95 |
| 9 | Compressor inlet temperature | 8.95 |
| 10 | Gas recycle temperature | 8.95 |
| 11 | Quencher outlet pressure | 7.64 |
| 12 | Separator inlet temperature | 6.74 |
| 13 | Reactor inlet pressure | 4.15 |
| 14 | Reactor outlet pressure | 4.09 |

Decision of key controlled variables using fixture point theorem (Reaction section)

Table 4.8 shows the result of fixture point; we found the first point which should be controlled is quencher outlet temperature because quencher outlet temperature has the most effect to other process variables. The second point should be controlled is reactor inlet temperature.

Composition variable tests are very hard to add imitation stream into the process simulation because addition pure component stream affect to flow rate variable so we consider indirect way by using the result from other variables test and evaluation affectation of each variable to composition variation. The rank of composition is show in table 4.9.

Use the fixture points for decision and selecting the controlled variables.

As step 1 the key parameters are quencher temperature, reactor inlet temperature, reactor outlet temperature and hydrogen to aromatic ratio in reactor inlet.

The fixture point ranking is shown in table 4.8. If we compare the result of fixture point with operation constraints, it takes clearly quencher temperature, reactor inlet and reactor outlet temperature which are the first set of controlled variables.

As step 3 we provide a key safety parameter, methane composition which should be controlled for prevent snowball effect. The fixture points imply methane composition content at separator vapor stream which should be fixed. (At the point has higher sensitivity).

The temperature at reactor outlet constraint is to maintain within 1300°F. From the steady-state simulation model, it can be seen that the reactor outlet temperature (1201.2°F) is well below 1300°F in order to make sure that the higher reactor outlet temperature (1271.3°F) is also below 1300°F from the fixture point test. The reactor outlet temperature may not be controlled by directly.

The primary key controlled variables (CVs) are

(1) Quencher outlet temperature
(2) Reactor inlet temperature
(3) Separator pressure
(4) Hydrogen to aromatic ratio
(5) Methane composition at separator overhead vapor

**Table 4.9** Ranks of key composition variables

| Ranking | Key composition variables | Variation |
|---|---|---|
| 1 | Hydrogen to aromatic ratio in reactor inlet stream | 7.28 |
| 2 | Hydrogen composition of separator vapor stream | 3.78 |
| 3 | Hydrogen composition of compressor inlet stream | 3.78 |
| 4 | Hydrogen composition of reactor outlet stream | 3.51 |
| 5 | Methane composition of separator vapor stream | 3.50 |
| 6 | Methane composition of compressor inlet stream | 3.49 |
| 7 | Hydrogen composition of quencher outlet stream | 3.41 |
| 8 | Methane composition of reactor outlet stream | 3.33 |
| 9 | Hydrogen composition of mixer outlet stream | 3.25 |
| 10 | Hydrogen composition of reactor inlet stream | 3.25 |
| 11 | Methane composition of quencher outlet stream | 3.16 |
| 12 | Methane composition of mixer outlet stream | 2.97 |
| 13 | Methane composition of reactor inlet stream | 2.97 |

**Table 4.10** Maximum Scale Gain between key process variables and manipulation.

| CVs | Gain | | | | |
|---|---|---|---|---|---|
| | V1 | V2 | V5 | V6 | Qfur |
| 1 | -0.0001 | 0.0015 | 0.0042 | **-0.0074** | 0.0193 |
| 2 | 0.0009 | -0.0003 | 0.0044 | -0.0065 | **0.0303** |
| 3 | **0.0179** | 0.0093 | -0.0065 | -0.0132 | 0.0852 |
| 4 | 0.0109 | **-0.0127** | -0.0090 | 0.0074 | -0.0304 |
| 5 | -0.0139 | 0.0132 | **0.0082** | -0.0127 | 0.0294 |

Note: 1= quencher outlet temperature 2= reactor inlet temperature 3= separator pressure
4= hydrogen to aromatic ratio 5= methane composition at separator overhead vapor

The major costs with gas recycle are compressor capital investment and compressor work, so this work we fixed the compressor power at nominal point.

Selection of manipulator for primary controlled variables

From the process knowledge and maximum scale gain between key process variables and manipulation variables (show in table 4.10), we can pair flows of cooling stream to quencher (V6) used to control the quencher outlet temperature. The reactor inlet temperature is controlled by furnace heat duty (direct action and fast response).

The hydrogen to aromatic ratio at the reactor inlet is maintained by toluene fresh feed stream (V2). One reason, we use the toluene fresh feed stream control hydrogen aromatic ratio because H2:Toluene approximate 1:5 so, if process use toluene 1 lbmole (1 lbmole x 1.14 $/lbmole=1.14$), it must use 5 lbmole of hydrogen (5 kgmole x 6.04 $/lbmole=30.2$). We can see toluene more expensive than hydrogen. The methane composition at separator overhead vapor stream is maintained by purge gas valve (V5).

Step 6 Energy management

To avoid heat removals from the thermal sinks and prevent propagation of thermal disturbance. Heat from the adiabatic reactor is carried in the effluent stream and is not removed from the process until it is dissipated to utility in the separator cooler. The temperature is fixed at separator inlet stream by cooler utility for heat removal and hydrogen separation condition.

Step 7 Establish remaining individual unit operations

Reaction section:

The objective in this step is to prevent the plant from accumulate or run away from desired operating point. Separator liquid level is manipulated by stabilizer feed valve. The pressure should be controlled somewhere in the reaction section. From fixture point ranking, the separator pressure should be controlled. Hydrogen fresh feed valve manipulate pressure at separator. Fresh toluene and fresh Hydrogen gas feed rate should be controlled for prevent drift of upstream. Toluene fresh feed valve and hydrogen fresh feed valve are manipulating the fresh toluene and fresh gas hydrogen feed rate.

Separation section:

First levels are controlled; the reboiler liquid level is controlled by bottom flow rate, condenser liquid level is controlled by distillate flow rate and exemption the stabilizer column. Condenser liquid level at stabilizer column is controlled by condenser heat duty because the distillate stream is a gas phase and fast dynamic response for pressure condenser control. Condenser pressure in product column and toluene column are controlled by condenser heat duty.

We use the steady-state data for distillation columns follow by Sigurd Skogestad and Antonio, 2006. They specify 6 values of composition variables for minimize economic loss at distillation column (flat utility usage).

Temperature control in distillation column is an effective means of maintaining composition control for column from a control and economic standpoint. We improved the fixture point theorem for selection tray. The major type of load disturbances in distillation columns is feed composition.

1. Stabilizer column

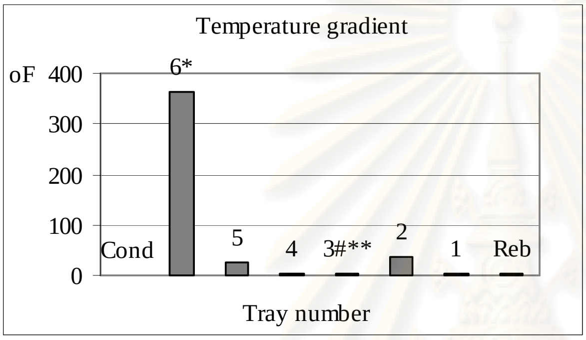


Figure 4.2 Temperature gradient

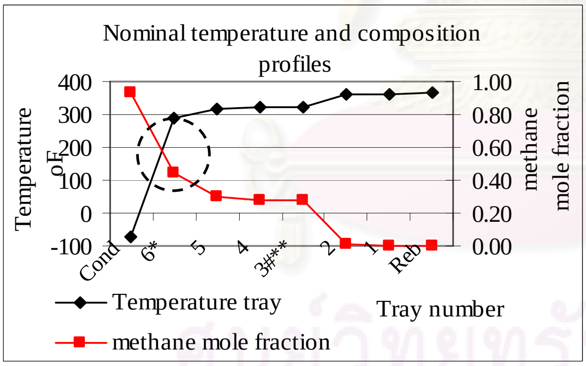


Figure 4.3 Nominal temperature and composition profiles

For the stabilizer, Figure 4.4 shows that the choice from a sensitive point of view would control temperature around stage 6 (TS6) since the temperature and methane composition sensitivity is higher at this location. The nominal temperature and methane composition profiles (Figure 4.3) show that the intersection between temperature and methane com-position around stage 6 namely temperature change the most affect to methane composition change. We use reboiler heat duty (qr1) as the manipulated variable.

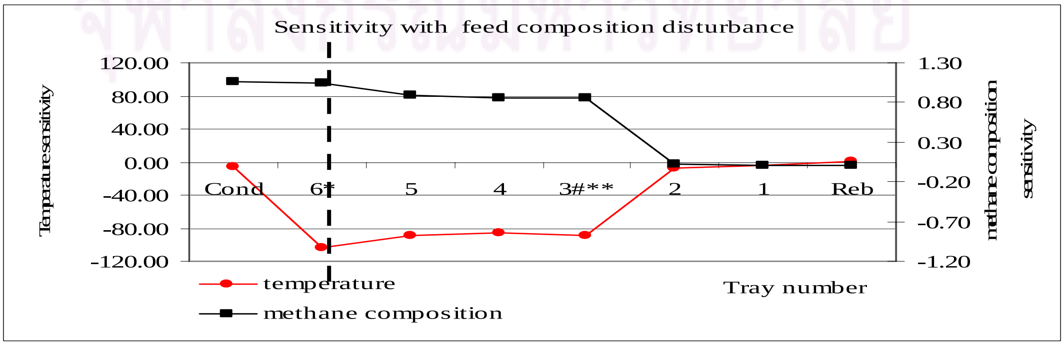


Figure 4.4 Temperature and composition sensitivity with feed composition disturbance

Note: Symbol; # is feed tray, * is Luyben controlled variable and ** is Antonio controlled variable.

2. Benzene column

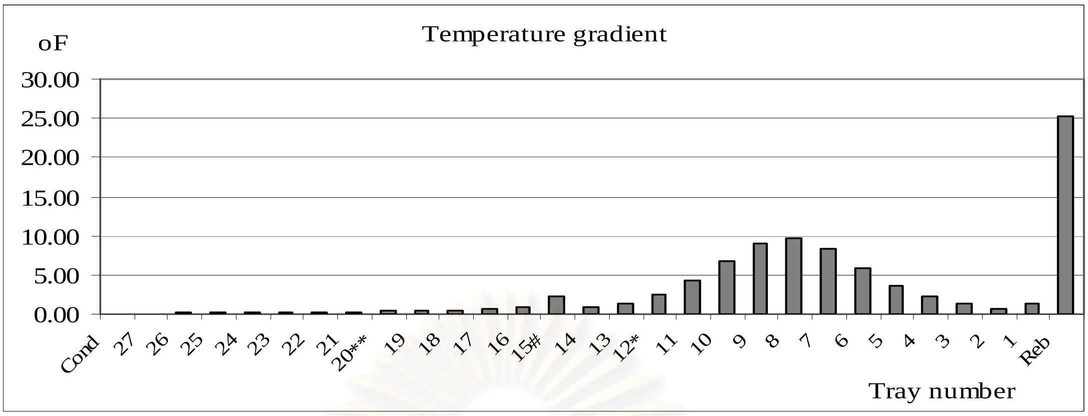


Figure 4.5 Temperature gradient

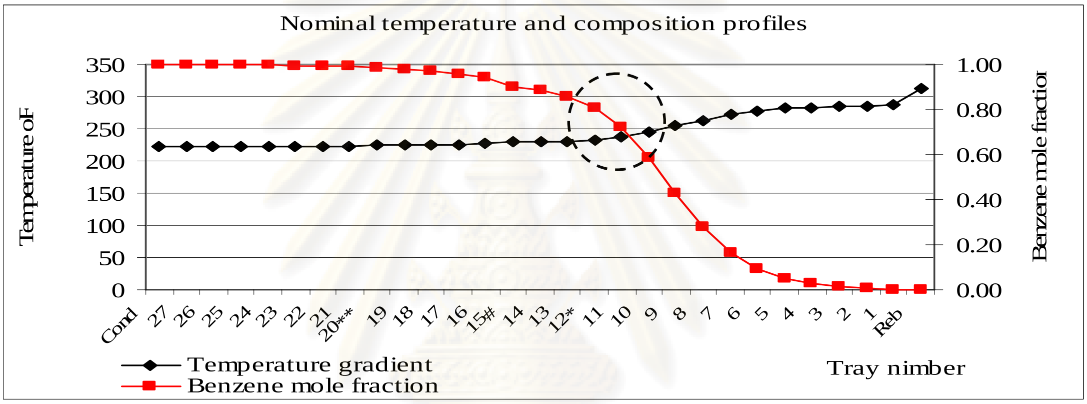


Figure 4.6 Nominal temperature and composition profiles

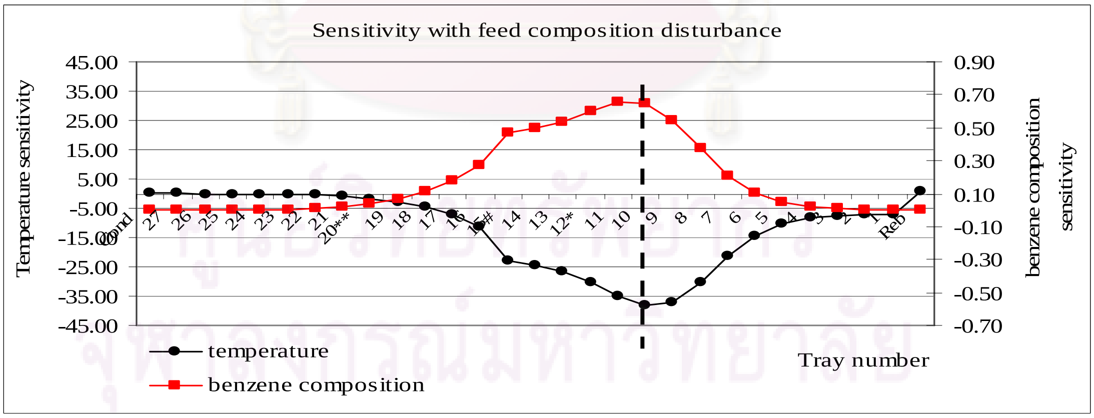


Figure 4.7 Temperature and composition sensitivity with feed composition disturbance

**Note:** Symbol; # is feed tray, * is Luyben controlled variable and ** is Antonio controlled variable.

For the product column, Figure 4.7 shows that the choice from a sensitive point of view would control temperature around stage 10 (TS10) since the temperature and benzene composition sensitivity is higher at this location. We use reboiler heat duty (qr2) as the manipulated variable.

3. Toluene column

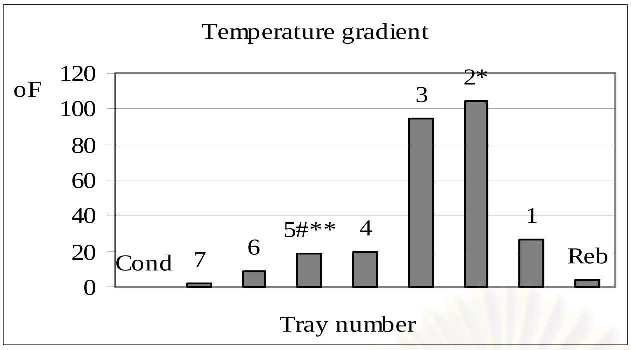


Figure 4.8 Temperature gradient

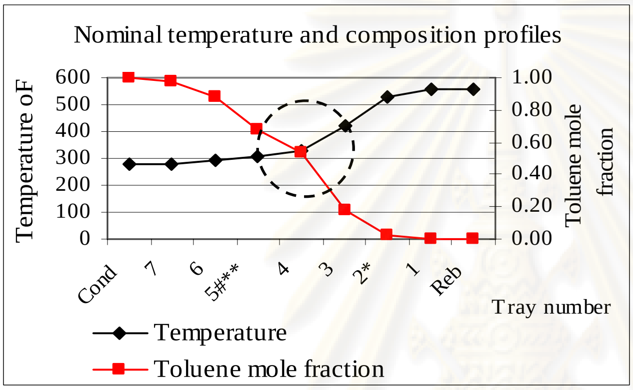


Figure 4.9 Nominal temperature and composition profiles

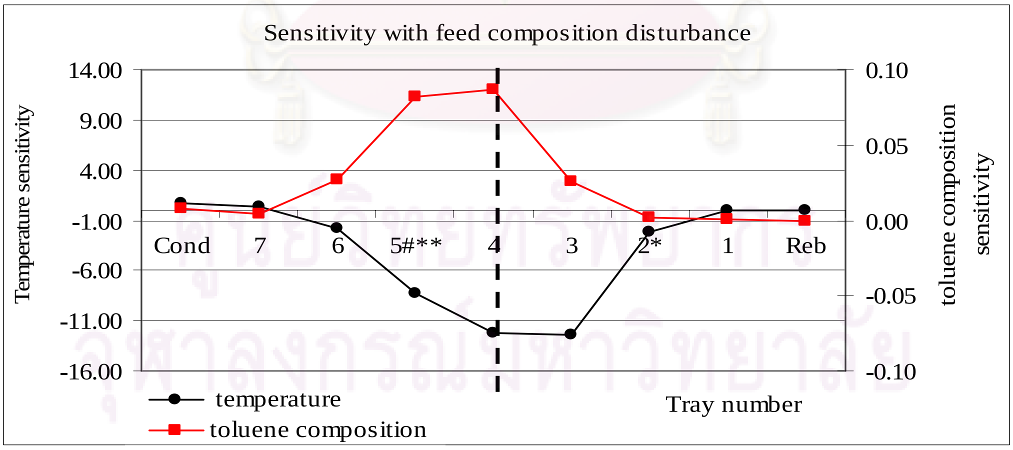


Figure 4.10 Temperature and composition sensitivity with feed composition disturbance

Note: Symbol; # is feed tray, * is Luyben controlled variable and ** is Antonio controlled variable.

For the toluene column, Figure 4.10 shows that the choice from a sensitive point of view would control temperature around stage 4 (TS4) since the temperature and benzene composition sensitivity is higher at this location. We use reboiler heat duty (qr3) as the manipulated variable.

### 4.3.2 Summary of loops control structure for REF1, REF2 and control structure CS1

| Controller | Controlled variables (CV) | Manipulated variable (MV) | | |
|---|---|---|---|---|
| | | REF1 | REF2 | CS1 |
| TC01 | Quencher outlet temperature | V6 | V6 | V6 |
| TC02 | Reactor inlet temperature | Qfur | Qfur | Qfur |
| TC03 | Separator inlet temperature | Qcooler | Qcooler | Qcooler |
| RC01 | Hydrogen to aromatic ratio at reactor inlet | Wkcomp | - | SP FC-02 |
| PC-RIN | Reactor inlet pressure | V5 | - | - |
| PC-SEP | Separator pressure | - | V1 | SP FC-01 |
| CC01 | Mixer outlet methane mole fraction | SP FC-01 | - | - |
| CC-RCH4 | Compressor inlet methane mole fraction | - | V5 | - |
| CC-GCH4 | Separator vapor methane mole fraction | - | - | V5 |
| CC02 | Quencher outlet toluene mole fraction | SP TC-02 | - | - |
| LC-SEP | Separator liquid level | V4 | V4 | V4 |
| LC1 | Reflux drum level of stabilizer column | qc1 | qc1 | qc1 |
| LC2 | Reflux drum level of benzene column | V13 | V13 | V13 |
| LC3 | Reflux drum level of toluene column | V10 | V10 | V10 |
| LRC1 | Reboiler sump level of stabilizer column | V12 | V12 | V12 |
| LRC2 | Reboiler sump level of benzene column | V14 | V14 | V14 |
| LRC3 | Reboiler sump level of toluene column | V15 | qr3 | V15 |
| PC1 | Condenser pressure of stabilizer column | V11 | V11 | V11 |
| PC2 | Condenser pressure of benzene column | qc2 | qc2 | qc2 |
| PC3 | Condenser pressure of toluene column | qc3 | qc3 | qc3 |
| C1 TS-3 | Temperature at tray 3 in stabilizer column | qr1 | - | - |
| C1 TS-6 | Temperature at tray 6 in stabilizer column | - | qr1 | qr1 |
| C2 TS-20 | Temperature at tray 20 in benzene column | qr2 | - | - |
| C2 TS-12 | Temperature at tray 12 in benzene column | - | qr2 | - |
| C2 TS-10 | Temperature at tray 10 in benzene column | - | - | qr2 |
| C3 TS-5 | Temperature at tray 5 in toluene column | Reflux rate | - | - |
| C3 TS-Avg | Average trays temperature ( tray 1-4 ) in toluene column | - | V15 | - |
| C3 TS-4 | Temperature at tray 4 in toluene column | - | - | qr3 |

| Controller | Controlled variables (CV) | Manipulated variable (MV) | | |
|---|---|---|---|---|
| | | REF1 | REF2 | CS1 |
| CC11 | Benzene mole fraction in distillate of stabilizer column | Reflux rate | - | - |
| CC12 | Methane mole fraction in bottoms of stabilizer column | SP C1 TS-3 | - | - |
| CC21 | Toluene mole fraction in distillate of benzene column | Reflux rate | - | - |
| CC22 | Benzene mole fraction in bottoms of benzene column | SP C2 TS-20 | - | - |
| CC31 | Biphenyl mole fraction in distillate of toluene column | SP C3-TS5 | - | - |
| CC32 | Toluene mole fraction in bottoms of toluene column | qr3 | - | - |
| FC01 | Fresh hydrogen feed flowrate | V1 | - | V1 |
| FC02 | Fresh toluene feed flowrate | V2 | - | V2 |
| FC-TOT | Total toluene feed flowrate | - | V2 | - |

### 4.3.3 Dynamic response of control structure CS1 compare with REF1 and REF2

The differences of this work with Antonio are (1) Araujo control reactor inlet pressure with purge valve and this work does not control but control pressure at separator pressure with fresh feed hydrogen , (2) Araujo control hydrogen to aromatic ratio with compressor power and this work we control it with fresh feed toluene , (3) Araujo prevent accumulation of methane by control methane composition at mixture stream with fresh feed hydrogen and this work we control methane composition at gas separator stream with purge valve., (4) Araujo control benzene composition by control toluene composition of distillation of benzene column ( $X_{D,tol}^{Ben}$ ) and control benzene composition of bottom of benzene column ( $X_{B,ben}^{ben}$ .) This work does not control purity of product by directly.

The differences of this work with Luyben are (1) Luyben does not control hydrogen to aromatic ratio, (2) Luyben control methane composition at gas recycle stream with purge valve (3) Luyben control separator pressure like this work.

Figure 4.14 shows the response to increase load disturbance of fresh feed methane composition from 0.03 to 0.05. The reaction section of this work, we can see hydrogen to aromatic ratio is smooth operation, reactor inlet pressure has a little decreasing but it can return to set-point within 1 hr and Xmet,mix has a little increasing but it can return to set-point within 1.3 hr and response of this work of Xmet,mix better than Araujo and Luyben.

Figure 4.15 shows the response to step increase quencher outlet temperature from 1150 °F to 1170 °F. The reaction section of this work, we can see hydrogen to aromatic ratio is smooth operation, reactor inlet pressure has a little offset and Xmet,mix has a little oscillation and less than Araujo.

Table 4.11 and Figure 4.16 show the IAE results for change in the disturbance of quencher outlet temperature and the IAE results for change in the methane mole fraction of fresh feed gas.

For change in the disturbance CS1 control structure is the most effective on compared with REF1 and REF2 reference.

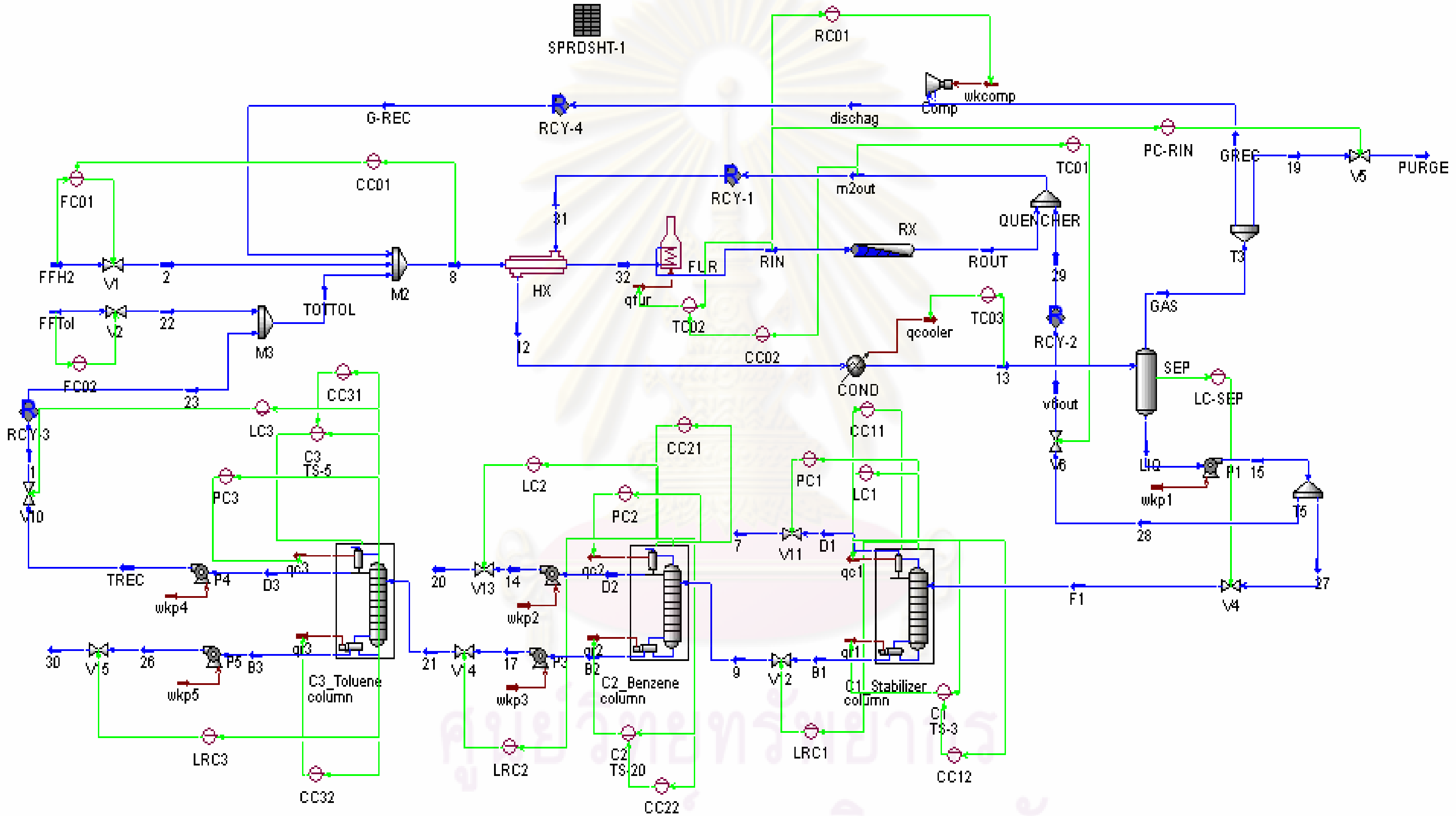


Figure 4.11 The Flowsheet of Simulation Hydrodealkylation (HDA) process of the Reference Control Structure 1(REF1) (Araujo et al.; 2006)

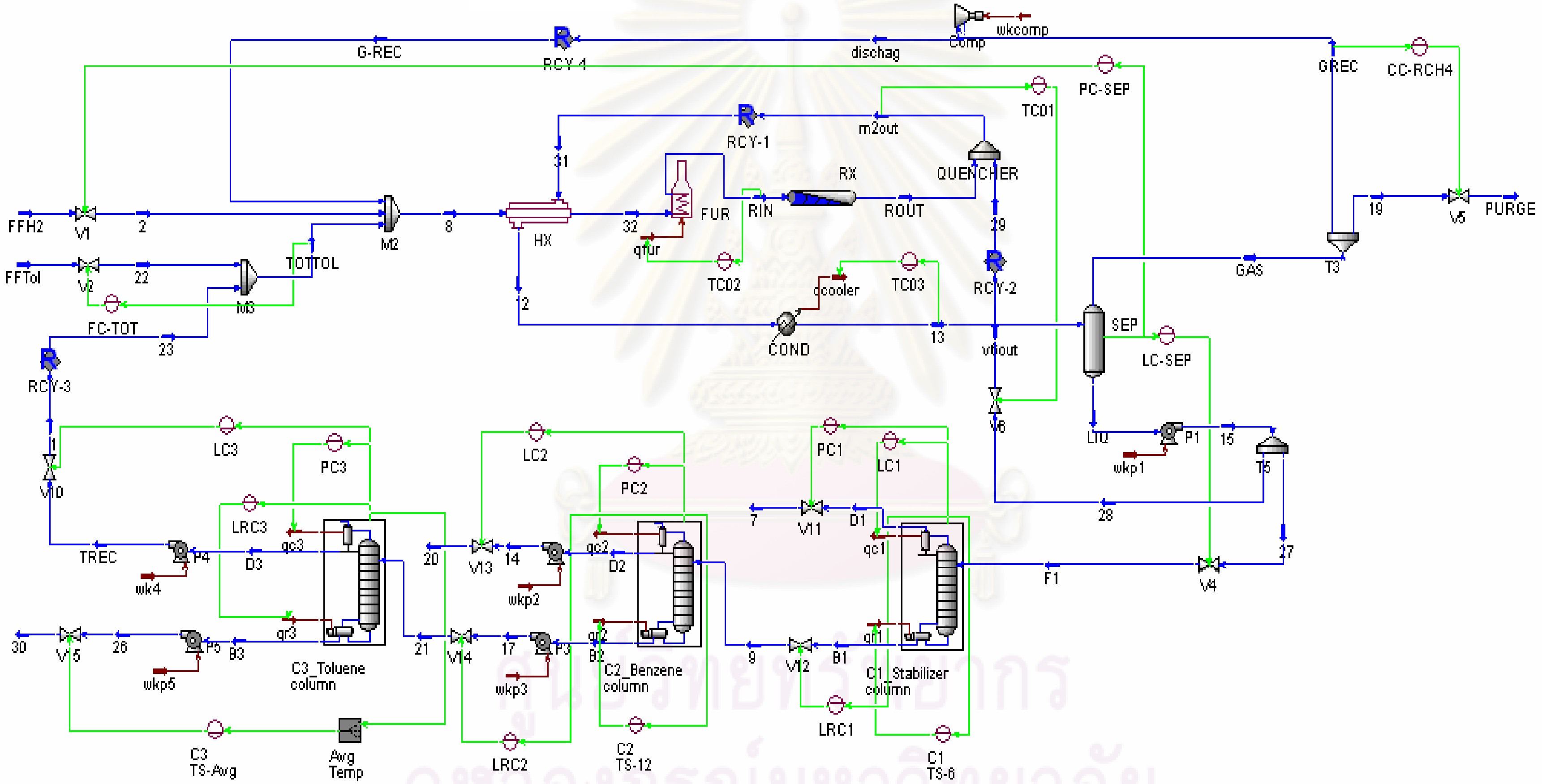


Figure 4.12 The Flowsheet of Simulation Hydrodealkylation (HDA) process of the Reference Control Structure 2(REF2) (Luyben; 1998)

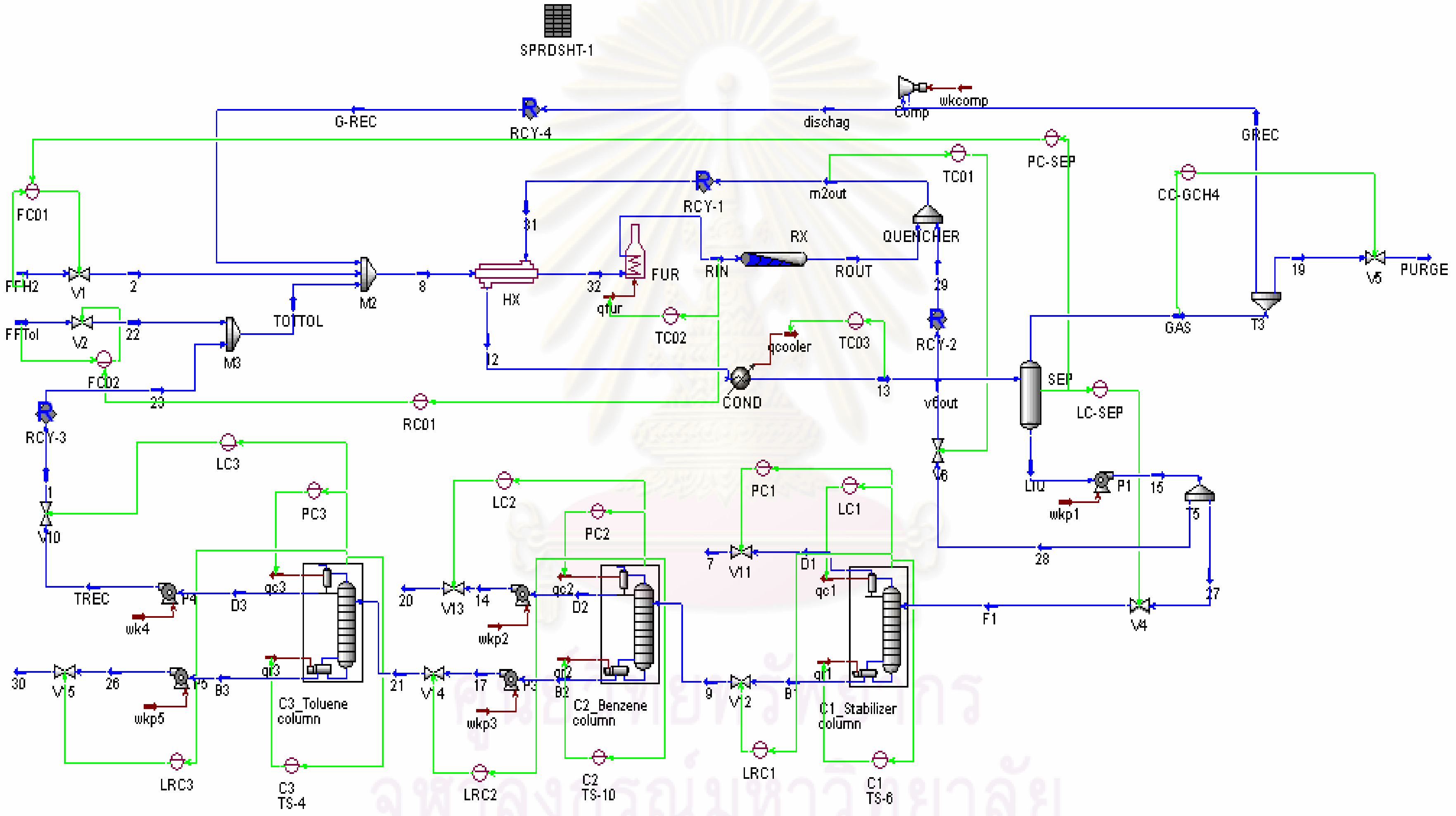


Figure 4.13 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed control structure 1 (CS1)

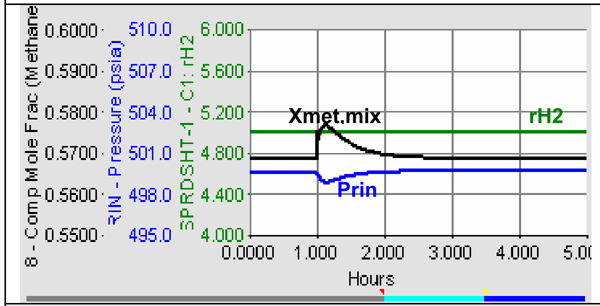
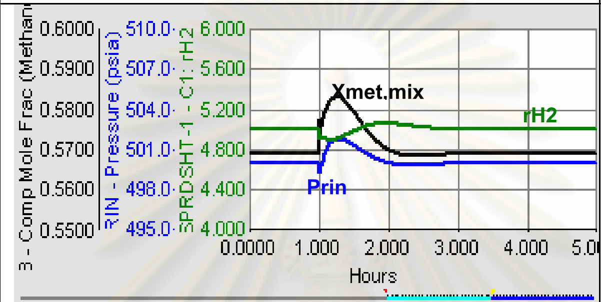
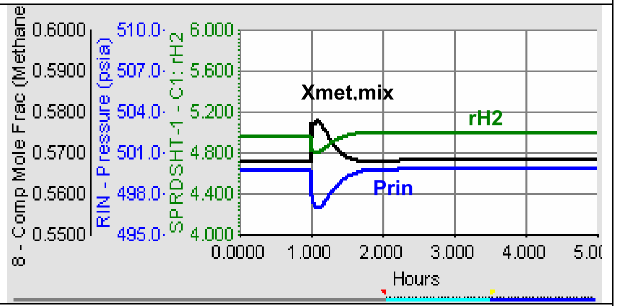
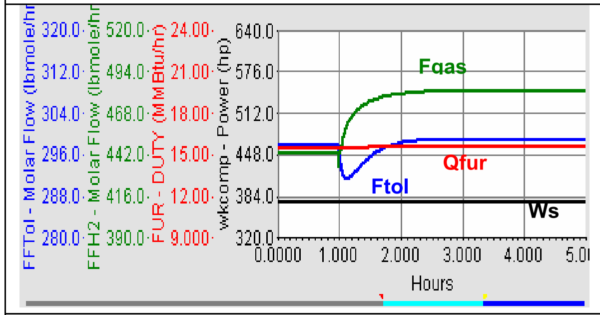
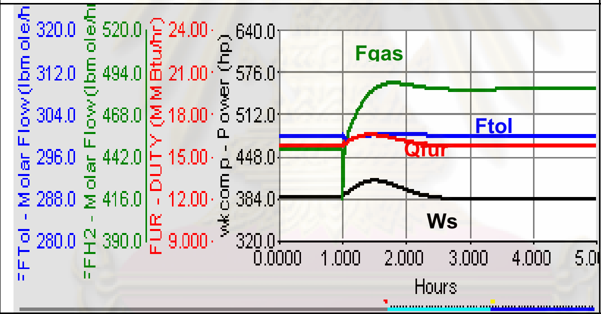
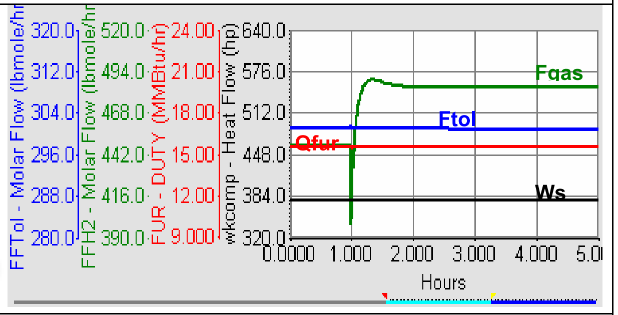
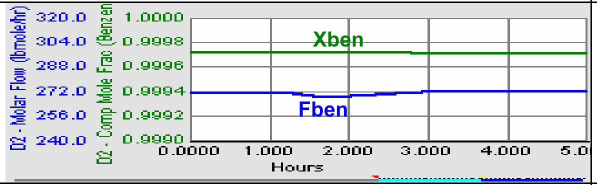
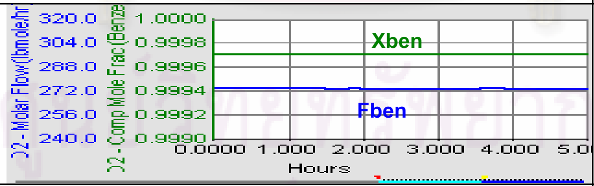
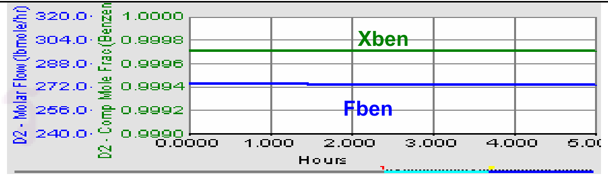
| This work (CS1) | Araujo et al.(2006) | Luyben (2002) |
|---|---|---|
|  |  |  |
| Reaction section | Reaction section | Reaction section |
|  |  |  |
| Manipulation in reaction section | Manipulation in reaction section | Manipulation in reaction section |
|  |  |  |
| Benzene product | Benzene product | Benzene product |

Figure 4.14 Comparison dynamic responses of step change in fresh gas feed rate methane mole fraction from 0.03 to 0.08 (increase 0.05) between: this work, Araujo et al.(2006) and Luyben's configuration.

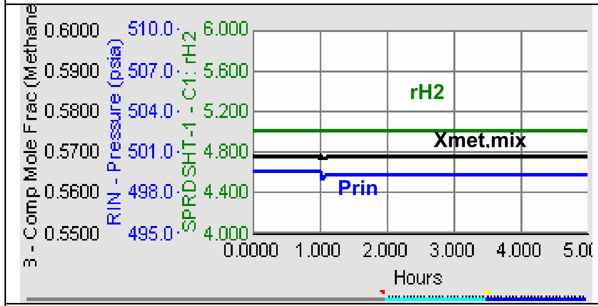
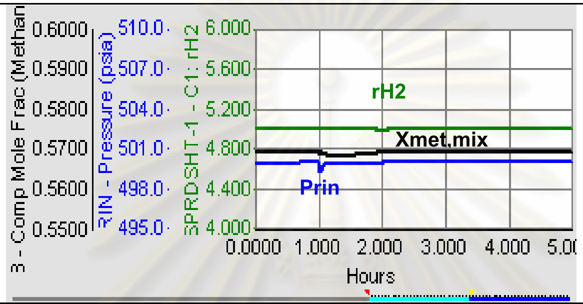
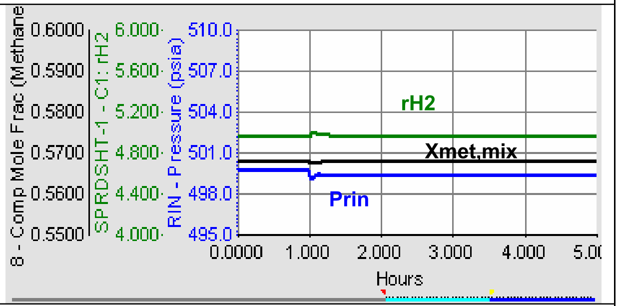
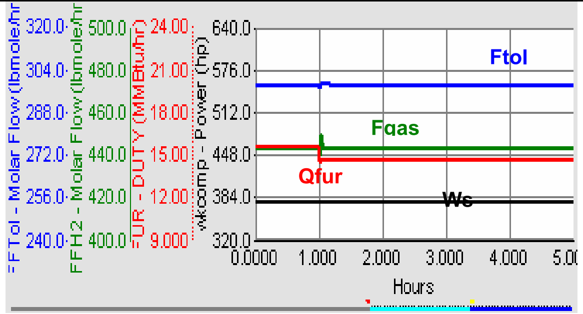
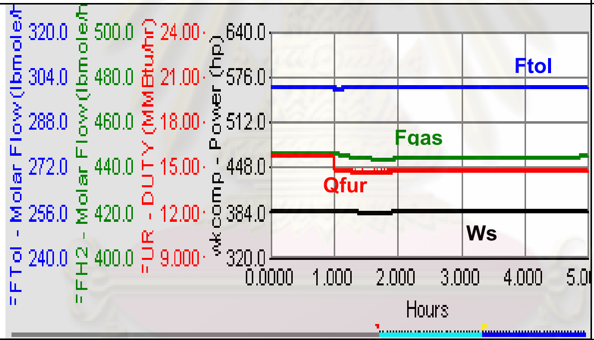
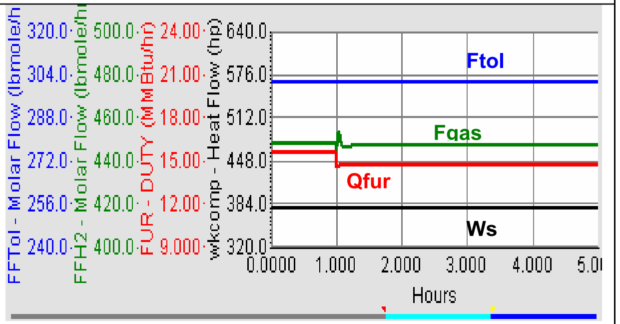
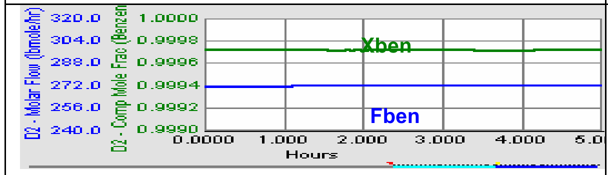
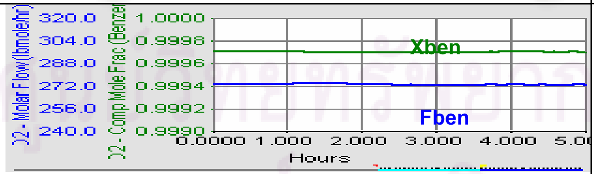
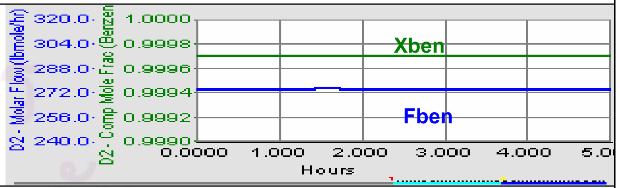
| This work (CS1) | Araujo et al.(2006) | Luyben (2002) |
|---|---|---|
|  |  |  |
| Reaction section | Reaction section | Reaction section |
|  |  |  |
| Manipulation in reaction section | Manipulation in reaction section | Manipulation in reaction section |
|  |  |  |
| Benzene product | Benzene product | Benzene product |

**Figure 4.15** Comparison dynamic responses of step change in quench outlet temperature from 1150 °F to 1170 °F (increase 20 °F) between: this work, Araujo et al.(2006) and Luyben's configuration.

**Table 4.11** The IAE results of loop control of the CS1 control structure compare with REF1 and REF2 references to change in the disturbance load.

| Disturbance = increase quencher outlet temperature | | | |
|---|---|---|---|
| CS | REF1 | REF2 | CS1 |
| Tquench | 1.051 | 0.975 | 0.974 |
| Trin | 2.657 | 0.167 | 0.175 |
| Psep | - | 1.139 | 0.861 |
| rH2 | 1.959 | - | 0.041 |
| Xmet,sep vap | - | - | 1.000 |
| Xmet,GREC | - | 1.000 | - |
| FFH2 | 1.699 | - | 0.301 |
| FFTOL | 1.852 | - | 0.148 |
| TSEP | 0.240 | 1.386 | 1.374 |
| Xmet,mix | 1.000 | - | - |
| Prin | 1.000 | - | - |
| Xtol,quench | 1.000 | - | - |
| Ftottol | - | 1.000 | - |
| SUM | 12.458 | 5.667 | 4.875 |

| Disturbance = increase methane mole fraction in fresh feed gas | | | |
|---|---|---|---|
| CS | REF1 | REF2 | CS1 |
| Tquench | 2.052 | 0.203 | 0.745 |
| Trin | 2.955 | 0.026 | 0.019 |
| Psep | - | 1.461 | 0.539 |
| rH2 | 1.952 | - | 0.048 |
| Xmet,sep vap | - | - | 1.000 |
| Xmet,GREC | 0.000 | 1.000 | - |
| FFH2 | 1.922 | - | 0.078 |
| FFTOL | 1.908 | - | 0.092 |
| TSEP | 1.125 | 0.470 | 1.405 |
| Xmet,mix | 1.000 | - | - |
| Prin | 1.000 | - | - |
| Xtol,quench | 1.000 | - | - |
| Ftottol | - | 1.000 | - |
| SUM | 14.913 | 4.160 | 3.926 |

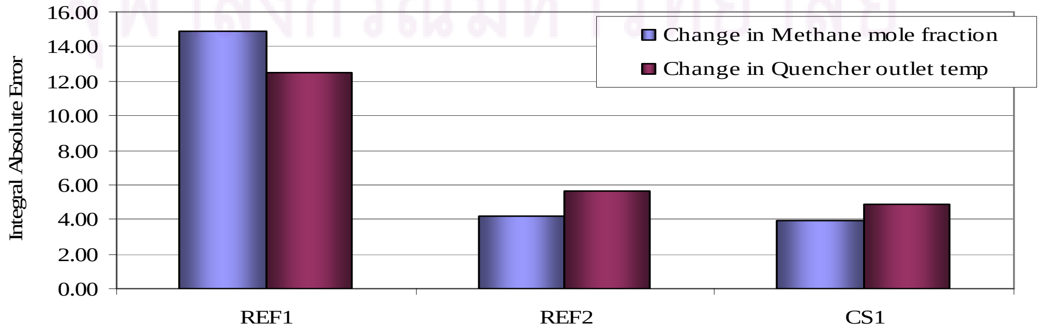


**Figure 4.16** The IAE results of change the methane mole fraction in fresh feed gas and change the quencher outlet temperature.

# CHAPTER V

# CONTROL STRUCTURE ALTERNATIVES

## 5.1 Selecting controlled output: Fixture point method.

The fixture point theorem is base on the idea of the most disturbed points must be satisfactorily controlled by giving them consideration before other controlled variables. The assumption can easily be used for selecting the primary controlled output. In chapter 4 shows a case study for the steps of control structure design and use the first set from fixture point for controlled variable in reaction section. The separation section we use heuristics for design the control configuration and use the fixture point for selection the tray temperature for purity control.

In practice, we can select controlled output from the next rank of variable (in the results of fixture point ranking). Therefore, we choose 3 sets of controlled variables to propose the fixture point that are given the appropriate set of controlled variables. The difference controlled variables shown in Table 5.1. The difference of SET1 and SET2 are position of methane mole fraction control. The difference of SET1 and SET3 are position of methane mole fraction control and pressure control (SET1 control separator pressure and SET2 control reactor inlet pressure).

In this section, we designed 5 control structures in reaction section and the separation section are the same control structure (see chapter 4 for separation section configuration). We use the maximum (scale) gain between manipulation and candidate key process variables for control configuration. The maximum (scale) gain for pairing the controlled variables with manipulated variables of control configurations (CS1-CS5) is shown in Table 5.2-5.4. Evaluate dynamic performance compare with reference control structure REF1 (Araujo et al., 2006) and REF2 (Luyben, 1998).

**Table 5.1** Controlled variables of SET1 to SET3

| Set | Number | Controlled variables |
|---|---|---|
| 1 | 1 | Quencher outlet temperature |
| | 2 | Reactor inlet temperature |
| | 3 | Separator pressure |
| | 4 | Hydrogen to aromatic ratio at reactor inlet stream |
| | 5 | Methane mole fraction in separator vapor stream |
| 2 | 1 | Quencher outlet temperature |
| | 2 | Reactor inlet temperature |
| | 3 | Separator pressure |
| | 4 | Hydrogen to aromatic ratio at reactor inlet stream |
| | **5** | **Methane mole fraction in mixer outlet stream** |
| 3 | 1 | Quencher outlet temperature |
| | 2 | Reactor inlet temperature |
| | **3** | **Reactor inlet pressure** |
| | 4 | Hydrogen to aromatic ratio at reactor inlet stream |
| | **5** | **Methane mole fraction in mixer outlet stream** |

**Table 5.2** The maximum (scale) gain for set 1

| | Rank | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| | CV | Tquench | Trin | P sep | rH2 | G-CH4 |
| | MV | y1 | y2 | y3 | y4 | y5 |
| 1 | V6 | -0.0074 | -0.0065 | -0.0132 | 0.0074 | -0.0127 |
| 2 | V1 | -0.0001 | 0.0009 | 0.0179 | 0.0109 | -0.0139 |
| 3 | V2 | 0.0015 | -0.0003 | 0.0093 | -0.0127 | 0.0132 |
| 4 | V5 | 0.0042 | 0.0044 | -0.0065 | -0.0090 | 0.0082 |
| 5 | qfur | 0.0193 | 0.0303 | 0.0852 | -0.0304 | 0.0294 |
| 6 | wkcomp | -0.0088 | -0.0113 | -0.0357 | 0.0184 | -0.0264 |

**Table 5.3** The maximum (scale) gain for set 2

| | Rank | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| | CV | Tquench | Trin | Psep | rH2 | 8-CH4 |
| | MV | y1 | y2 | y3 | y4 | y5 |
| 1 | V6 | -0.0074 | -0.0065 | -0.0132 | 0.0074 | -0.0111 |
| 2 | V1 | -0.0001 | 0.0009 | 0.0179 | 0.0109 | -0.0118 |
| 3 | V2 | 0.0015 | -0.0003 | 0.0093 | -0.0127 | 0.0102 |
| 4 | V5 | 0.0042 | 0.0044 | -0.0065 | -0.0090 | 0.0056 |
| 5 | qfur | 0.0193 | 0.0303 | 0.0852 | -0.0304 | 0.0263 |
| 6 | wkcomp | -0.0088 | -0.0113 | -0.0357 | 0.0184 | -0.0215 |

**Table 5.4** The maximum (scale) gain for set 3

| | Rank | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| | CV | Tquench | Trin | Prin | rH2 | 8-CH4 |
| | MV | y1 | y2 | y3 | y4 | y5 |
| 1 | V6 | -0.0074 | -0.0065 | -0.0127 | 0.0074 | -0.0111 |
| 2 | V1 | -0.0001 | 0.0009 | 0.0173 | 0.0109 | -0.0118 |
| 3 | V2 | 0.0015 | -0.0003 | 0.0093 | -0.0127 | 0.0102 |
| 4 | V5 | 0.0042 | 0.0044 | -0.0069 | -0.0090 | 0.0056 |
| 5 | qfur | 0.0193 | 0.0303 | 0.0788 | -0.0304 | 0.0263 |
| 6 | wkcomp | -0.0088 | -0.0113 | -0.0311 | 0.0184 | -0.0215 |

**Table 5.5** Alternative schemes for SET 1- SET 3

| Scheme | Pairing (CV,MV) | Note |
|---|---|---|
| CS1 | [(1,1) (2,5) (3,2) (4,3) (5,4)] | work of compressor is fixed |
| CS2 | [(1,1) (2,5) (3,4) (4,3) (5,2)] | |
| CS3 | [(1,1) (2,5) (3,6) (4,2) (5,4)] | work of compressor is manipulation |
| CS4 | [(1,1) (2,5) (3,2) (4,6) (5,4)] | |
| CS5 | [(1,1) (2,5) (3,4) (4,6) (5,2)] | |

**Table 5.6** Control configurations of CS1- CS5 for SET 1-SET 3 (Reaction section)

| Controlled variables (CV) | Manipulated variable (MV) | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| SET1 | | | | | |
| Quencher outlet temperature | V6 | V6 | V6 | V6 | V6 |
| Reactor inlet temperature | Qfur | Qfur | Qfur | Qfur | Qfur |
| Hydrogen to aromatic ratio at reactor inlet | SP FC-02 | SP FC-02 | SP FC-01 | Wkcomp | Wkcomp |
| Reactor inlet pressure | - | - | - | - | - |
| Separator pressure | SP FC-01 | V5 | Wkcomp | SP FC-01 | V5 |
| Mixer outlet methane mole fraction | - | - | - | - | - |
| Separator vapor methane mole fraction | V5 | SP FC-01 | V5 | V5 | SP FC-01 |
| SET2 | | | | | |
| Quencher outlet temperature | V6 | V6 | V6 | V6 | V6 |
| Reactor inlet temperature | Qfur | Qfur | Qfur | Qfur | Qfur |
| Hydrogen to aromatic ratio at reactor inlet | SP FC-02 | SP FC-02 | SP FC-01 | Wkcomp | Wkcomp |
| Reactor inlet pressure | - | - | - | - | - |
| Separator pressure | SP FC-01 | V5 | Wkcomp | SP FC-01 | V5 |
| Mixer outlet methane mole fraction | V5 | SP FC-01 | V5 | V5 | SP FC-01 |
| Separator vapor methane mole fraction | - | - | - | - | - |
| SET3 | | | | | |
| Quencher outlet temperature | V6 | V6 | V6 | V6 | V6 |
| Reactor inlet temperature | Qfur | Qfur | Qfur | Qfur | Qfur |
| Hydrogen to aromatic ratio at reactor inlet | SP FC-02 | SP FC-02 | SP FC-01 | Wkcomp | Wkcomp |
| Reactor inlet pressure | SP FC-01 | V5 | Wkcomp | SP FC-01 | V5 |
| Separator pressure | - | - | - | - | - |
| Mixer outlet methane mole fraction | V5 | SP FC-01 | V5 | V5 | SP FC-01 |
| Separator vapor methane mole fraction | - | - | - | - | - |

## 5.2 Evaluation of the dynamic performance

The estimation of the minimum achievable variance of SISO controlled variable from “normal” closed- loop data. Since then, minimum variance control has been widely used as a benchmark for assessing control loop performance. However, minimum variance control based performance assessment methods cannot adequately evaluate the performance for controllers with constraints explicitly incorporated or for controllers where transient response and deterministic disturbance regulation are concerned. For assessing constrained control loop performance the proposed dynamic performance index is focused on time related characteristics of the controller’s response to set-point changes or deterministic disturbances. There exist several candidate performance measures such as settling time and integral absolute error (IAE). Integral absolute error is widely used for the formulation of a dynamic performance as written below:

$$IAE = \int |\varepsilon(t)| dt$$

In this study, IAE method is used to evaluate the dynamic performance of the designed control system.

### 5.2.1 Evaluation of the dynamic performance for CS1-CS5 of controlled variables SET1-SET3.

Table 5.7a and 5.7b show the IAE results of control loops for the change in step increase of quencher outlet temperature in HDA process and the IAE results of control loops for the disturbance loads of methane mole fraction in fresh feed gas in HDA process respectively.

For the step increase the quencher outlet temperature from 1150 °F to 1170 °F, the control structure 2 (CS2) of SET3 is the most effective on compared with the others. The controlled variables of SET1 and SET2 are the best set on compared with all control structures (CS1-CS5).

For the change in the disturbance loads of methane mole fraction of fresh feed gas, the control structure 2 (CS2) of SET3 is the most effective on compared with the others. The controlled variables of SET1 are the best set on compared with all control structures (CS1-CS5).

As can be seen that the control structure 2 (CS2) is the most effective on compared with CS1 (work compressor is fixed) and the control structure 5 (CS5) is the most effective on compared with CS3-CS5 (work of compressor is used).

**Table 5.7a** The IAE results of the control loops for each set to a change in quencher outlet temperature.

| | SET 1 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quencher Temp. | 0.999 | 0.990 | 0.994 | 1.010 | 1.007 |
| Reactor inlet Temp. | 1.010 | 0.975 | 1.010 | 1.003 | 1.002 |
| Separator Pressure | 0.900 | 0.984 | 1.474 | 0.921 | 0.722 |
| rH2 | 0.557 | 0.279 | 2.069 | 1.250 | 0.846 |
| Methane in Gas | 0.810 | 0.889 | 1.231 | 1.261 | 0.809 |
| FFH2 | 1.537 | 0.344 | 1.236 | 1.559 | 0.324 |
| FFTOL | 0.193 | 0.176 | 2.445 | 1.243 | 0.942 |
| Separator Temp. | 0.974 | 0.974 | 1.017 | 1.018 | 1.016 |
| SUM | 6.980 | 5.610 | 11.477 | 9.267 | 6.667 |

| | SET 2 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quencher Temp. | 0.999 | 0.990 | 0.991 | 1.011 | 1.009 |
| Reactor inlet Temp. | 1.012 | 0.973 | 1.030 | 0.983 | 1.002 |
| Separator Pressure | 0.800 | 1.124 | 1.333 | 0.845 | 0.899 |
| rH2 | 0.572 | 0.296 | 1.982 | 1.259 | 0.891 |
| FFH2 | 1.502 | 0.370 | 1.228 | 1.540 | 0.361 |
| FFTOL | 0.192 | 0.183 | 2.519 | 1.169 | 0.936 |
| Separator Temp. | 0.971 | 0.973 | 1.018 | 1.018 | 1.020 |
| Methane in mixer | 1.059 | 0.732 | 1.107 | 1.470 | 0.632 |
| SUM | 7.107 | 5.640 | 11.209 | 9.295 | 6.750 |

| | SET 3 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quencher Temp. | 0.994 | 0.988 | 0.991 | 1.017 | 1.010 |
| Reactor inlet Temp. | 0.973 | 0.954 | 1.018 | 1.060 | 0.996 |
| rH2 | 0.534 | 0.238 | 1.522 | 1.921 | 0.785 |
| FFH2 | 0.891 | 0.571 | 1.978 | 1.080 | 0.480 |
| FFTOL | 0.174 | 0.169 | 2.205 | 1.317 | 1.135 |
| Separator Temp. | 0.966 | 0.965 | 1.026 | 1.026 | 1.017 |
| Methane in mixer | 0.896 | 0.424 | 1.780 | 1.759 | 0.142 |
| Reactor inlet Pressure | 0.721 | 0.818 | 1.749 | 0.969 | 0.743 |
| SUM | 6.149 | 5.126 | 12.269 | 10.148 | 6.308 |

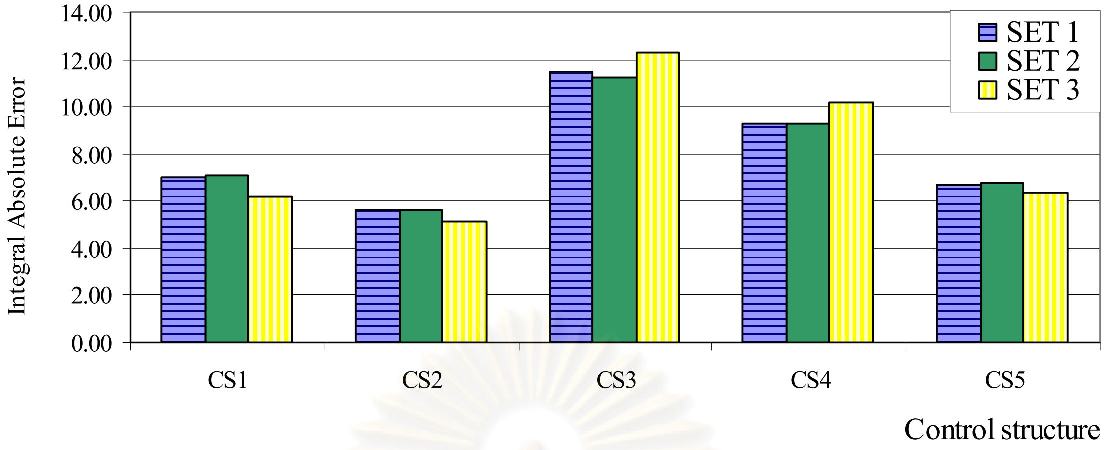


**Figure 5.1** The IAE results of control loop to a change the quencher outlet temperature.

Figure 5.1 shows the IAE results of the control loop a change in quencher outlet temperature, can be seen that SET1 and SET2 have the same results.

**Table 5.7b** The IAE results of the control loop for each set to a change in methane mole fraction of fresh feed gas.

| | SET 1 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quencher Temp. | 1.121 | 0.810 | 1.081 | 1.123 | 0.865 |
| Reactor inlet Temp. | 0.212 | 0.219 | 1.401 | 1.744 | 1.424 |
| Separator Pressure | 0.932 | 1.078 | 0.987 | 0.925 | 1.079 |
| rH2 | 0.536 | 0.435 | 1.001 | 1.778 | 1.251 |
| Methane in Gas | 1.052 | 0.934 | 1.054 | 1.046 | 0.914 |
| FFH2 | 0.888 | 0.875 | 1.034 | 1.026 | 1.177 |
| FFTOL | 0.100 | 0.062 | 1.683 | 1.348 | 1.808 |
| Separator Temp. | 0.450 | 0.285 | 1.418 | 1.589 | 1.257 |
| SUM | 5.290 | 4.698 | 9.658 | 10.580 | 9.775 |

| SET 2 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quencher Temp. | 1.138 | 0.782 | 1.170 | 1.066 | 0.843 |
| Reactor inlet Temp. | 0.243 | 0.129 | 1.489 | 1.722 | 1.417 |
| Separator Pressure | 0.970 | 1.094 | 0.889 | 0.962 | 1.085 |
| rH2 | 0.530 | 0.416 | 1.154 | 1.689 | 1.211 |
| FFH2 | 0.907 | 0.898 | 1.031 | 1.000 | 1.165 |
| FFTOL | 0.102 | 0.042 | 1.769 | 1.286 | 1.802 |
| Separator Temp. | 0.477 | 0.253 | 1.446 | 1.549 | 1.276 |
| Methane in mixer | 1.053 | 0.934 | 1.047 | 1.045 | 0.921 |
| SUM | 5.420 | 4.548 | 9.995 | 10.318 | 9.719 |

| SET 3 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quencher Temp. | 1.156 | 0.619 | 1.145 | 1.332 | 0.747 |
| Reactor inlet Temp. | 0.297 | 0.145 | 1.375 | 1.957 | 1.225 |
| rH2 | 0.513 | 0.339 | 1.009 | 2.142 | 0.996 |
| FFH2 | 0.788 | 0.787 | 1.554 | 0.821 | 1.050 |
| FFTOL | 0.137 | 0.047 | 1.987 | 0.887 | 1.943 |
| Separator Temp. | 0.510 | 0.207 | 1.429 | 1.755 | 1.099 |
| Methane in mixer | 1.037 | 0.910 | 1.104 | 1.057 | 0.892 |
| Reactor inlet pressure | 0.942 | 1.075 | 0.993 | 0.944 | 1.045 |
| SUM | 5.379 | 4.130 | 10.597 | 10.896 | 8.997 |

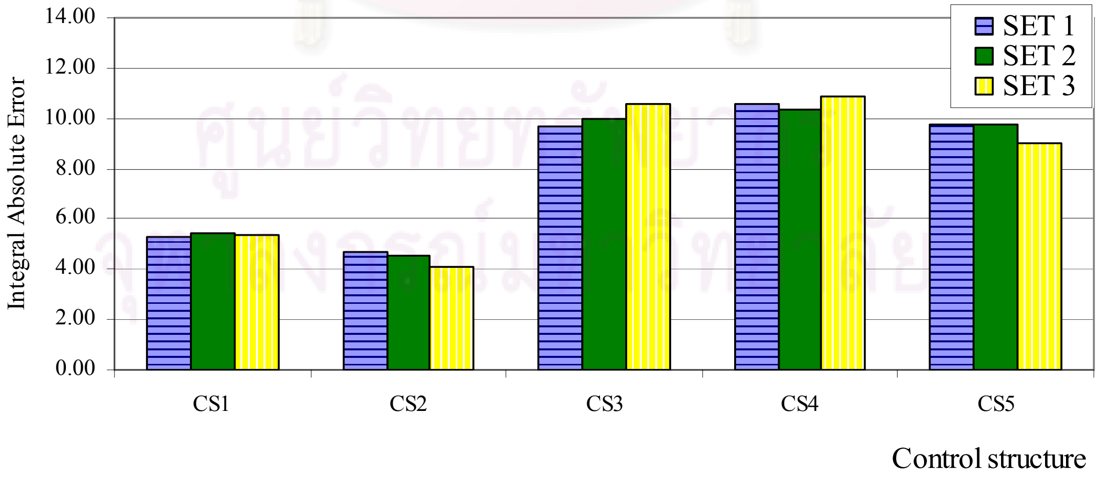


Figure 5.2 The IAE results of control loop to a change the methane mole fraction in fresh feed gas.

Figure 5.2 shows the IAE results of the control loop to a change in methane mole fraction of fresh feed gas, can be seen that SET1, SET2 and SET3 have the same results.

Table 5.8a and 5.8b show the IAE results of all control variables for the change in step increase of quencher outlet temperature in HDA process and the IAE results of all control variables for the disturbance loads of methane mole fraction in fresh feed gas in HDA process respectively.

For the step increase of set-point of quencher outlet temperature from 1150 oF to 1170 oF, the control structure 5 (CS5) of SET2 is the most effective on compared with the others. The SET2 is the best set on compared with all control structures (CS1-CS5).

For the change in the disturbance loads of methane mole fraction of fresh feed gas, the control structure 2 (CS2) of SET2 is the most effective on compared with the others. The SET2 are the best set on compared with all control structures (CS1-CS5).

As can be seen that the control structure 2 (CS2) is the most effective on compared with CS1 (work compressor is fixed) and the control structure 5 (CS5) is the most effective on compared with CS3-CS5 (work of compressor is used).

**Table 5.8a** The IAE results of considerate controlled variables (SET1-SET3) for CS1-CS5 to a change in quencher outlet temperature.

| | SET 1 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quench Temp. | 0.999 | 0.990 | 0.994 | 1.011 | 1.007 |
| Reactor inlet Temp. | 1.010 | 0.976 | 1.010 | 1.003 | 1.002 |
| Separator Pressure | 0.017 | 0.019 | 0.029 | 0.018 | 0.014 |
| rH2 | 0.579 | 0.290 | 2.151 | 1.300 | 0.879 |
| Methane in Gas | 0.331 | 0.363 | 0.503 | 0.515 | 0.330 |
| FFH2 | 1.733 | 0.388 | 1.394 | 1.758 | 0.365 |
| FFTOL | 0.194 | 0.176 | 2.453 | 1.247 | 0.945 |
| TSEP | 0.977 | 0.977 | 1.020 | 1.021 | 1.019 |
| Methane in mixer | 2.031 | 1.651 | 1.972 | 2.013 | 1.547 |
| Reactor inlet Pressure | 1.421 | 1.420 | 1.530 | 1.528 | 1.536 |
| Toluene in quencher outlet | 0.947 | 0.947 | 0.996 | 0.996 | 0.998 |
| Total Toluene Flowrate | 1.521 | 1.518 | 0.465 | 0.435 | 0.330 |
| SUM | 11.760 | 9.713 | 14.516 | 12.845 | 9.974 |

| SET 2 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quench Temp. | 0.998 | 0.990 | 0.990 | 1.010 | 1.009 |
| Reactor inlet Temp. | 1.013 | 0.974 | 1.031 | 0.984 | 1.003 |
| Separator Pressure | 0.014 | 0.019 | 0.023 | 0.015 | 0.016 |
| rH2 | 0.503 | 0.260 | 1.744 | 1.108 | 0.784 |
| Methane in Gas | 1.641 | 1.759 | 1.167 | 1.330 | 1.305 |
| FFH2 | 1.627 | 0.401 | 1.331 | 1.669 | 0.391 |
| FFTOL | 0.182 | 0.173 | 2.377 | 1.103 | 0.883 |
| TSEP | 0.974 | 0.976 | 1.022 | 1.021 | 1.023 |
| Methane in mixer | 0.406 | 0.281 | 0.424 | 0.563 | 0.242 |
| Reactor inlet Pressure | 1.421 | 1.420 | 1.540 | 1.538 | 1.535 |
| Toluene in quencher outlet | 0.952 | 0.952 | 1.004 | 1.005 | 1.004 |
| Total Toluene Flowrate | 1.668 | 1.662 | 0.462 | 0.430 | 0.459 |
| SUM | 11.399 | 9.866 | 13.115 | 11.777 | 9.653 |

| SET 3 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quench Temp. | 0.995 | 0.988 | 0.992 | 1.018 | 1.010 |
| Reactor inlet Temp. | 0.972 | 0.952 | 1.016 | 1.058 | 0.995 |
| Separator Pressure | 2.683 | 2.670 | 3.156 | 3.182 | 3.126 |
| rH2 | 0.577 | 0.257 | 1.645 | 2.076 | 0.848 |
| Methane in Gas | 1.118 | 1.053 | 1.471 | 1.442 | 0.675 |
| FFH2 | 0.703 | 0.450 | 1.560 | 0.851 | 0.379 |
| FFTOL | 0.183 | 0.179 | 2.323 | 1.387 | 1.195 |
| TSEP | 0.960 | 0.959 | 1.020 | 1.019 | 1.011 |
| Methane in mixer | 0.693 | 0.328 | 1.378 | 1.361 | 0.110 |
| Reactor inlet Pressure | 0.016 | 0.018 | 0.039 | 0.022 | 0.017 |
| Toluene in quencher outlet | 0.980 | 0.979 | 1.082 | 1.083 | 1.074 |
| Total Toluene Flowrate | 2.918 | 2.817 | 0.155 | 0.135 | 0.025 |
| SUM | 12.798 | 11.650 | 15.836 | 14.634 | 10.465 |

Figure 5.3 and 5.4 show the IAE results of considerate controlled variables of every set for the change in quencher outlet temperature and the change in methane mole fraction of fresh feed gas respectively.

The SET2 gives the best set of controlled variables because the IAE results of loops control plus loops which no control are smaller than SET1 and SET3 in every control structures.

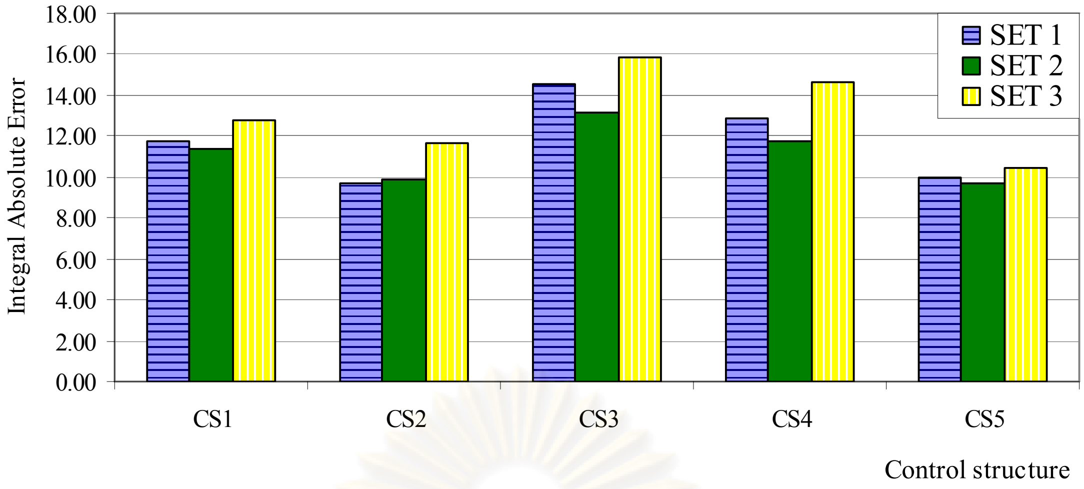


**Figure 5.3** The IAE results of considerate controlled variables to a change the quencher outlet temperature.

**Table 5.8b** The IAE results of considerate controlled variables (SET1-SET3) for CS1-CS5 to a change in methane mole fraction of fresh feed gas.

| | SET 1 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| Quench Temp. | 1.192 | 0.861 | 1.149 | 1.194 | 0.920 |
| Reactor inlet Temp. | 0.228 | 0.235 | 1.506 | 1.875 | 1.531 |
| Separator Pressure | 0.532 | 0.615 | 0.564 | 0.528 | 0.616 |
| rH2 | 0.563 | 0.458 | 1.053 | 1.870 | 1.316 |
| Methane in Gas | 1.006 | 0.893 | 1.008 | 1.000 | 0.874 |
| FFH2 | 0.868 | 0.856 | 1.011 | 1.003 | 1.150 |
| FFTOL | 0.112 | 0.069 | 1.886 | 1.511 | 2.026 |
| TSEP | 0.477 | 0.302 | 1.503 | 1.684 | 1.333 |
| Methane in mixer | 1.104 | 0.976 | 1.239 | 1.245 | 1.092 |
| Reactor inlet Pressure | 1.476 | 1.769 | 0.903 | 0.348 | 1.090 |
| Toluene in quencher outlet | 1.156 | 1.070 | 1.035 | 1.087 | 0.929 |
| Total Toluene Flowrate | 2.268 | 2.158 | 0.275 | 0.302 | 0.196 |
| SUM | 10.982 | 10.263 | 13.132 | 13.649 | 13.074 |

SET 2

| | CS1 | CS2 | CS3 | CS4 | CS5 |
|---|---|---|---|---|---|
| Quench Temp. | 1.039 | 0.714 | 1.069 | 0.974 | 0.770 |
| Reactor inlet Temp. | 0.217 | 0.116 | 1.332 | 1.541 | 1.267 |
| Separator Pressure | 0.529 | 0.597 | 0.485 | 0.525 | 0.592 |
| rH2 | 0.478 | 0.375 | 1.041 | 1.523 | 1.092 |
| Methane in Gas | 1.027 | 0.930 | 1.104 | 1.066 | 0.984 |
| FFH2 | 0.858 | 0.850 | 0.976 | 0.946 | 1.103 |
| FFTOL | 0.096 | 0.039 | 1.669 | 1.213 | 1.700 |
| TSEP | 0.431 | 0.228 | 1.307 | 1.399 | 1.153 |
| Methane in mixer | 0.972 | 0.863 | 0.967 | 0.964 | 0.851 |
| Reactor inlet Pressure | 1.462 | 1.747 | 0.722 | 0.278 | 0.959 |
| Toluene in quencher outlet | 1.162 | 1.082 | 0.827 | 0.866 | 0.729 |
| Total Toluene Flowrate | 2.156 | 2.053 | 0.254 | 0.271 | 0.225 |
| SUM | 10.428 | 9.594 | 11.751 | 11.566 | 11.424 |

SET 3

| | CS1 | CS2 | CS3 | CS4 | CS5 |
|---|---|---|---|---|---|
| Quench Temp. | 1.184 | 0.634 | 1.172 | 1.364 | 0.764 |
| Reactor inlet Temp. | 0.305 | 0.150 | 1.417 | 2.017 | 1.263 |
| Separator Pressure | 2.706 | 2.454 | 1.276 | 1.959 | 1.023 |
| rH2 | 0.536 | 0.355 | 1.056 | 2.242 | 1.042 |
| Methane in Gas | 1.019 | 0.921 | 1.126 | 1.050 | 0.991 |
| FFH2 | 0.847 | 0.847 | 1.672 | 0.884 | 1.130 |
| FFTOL | 0.128 | 0.044 | 1.858 | 0.829 | 1.818 |
| TSEP | 0.528 | 0.215 | 1.481 | 1.819 | 1.139 |
| Methane in mixer | 0.980 | 0.861 | 1.043 | 0.999 | 0.843 |
| Reactor inlet Pressure | 0.800 | 0.913 | 0.844 | 0.802 | 0.888 |
| Toluene in quencher outlet | 1.251 | 1.122 | 0.930 | 1.016 | 0.737 |
| Total Toluene Flowrate | 2.122 | 1.960 | 0.273 | 0.301 | 0.184 |
| SUM | 12.408 | 10.474 | 14.151 | 15.282 | 11.822 |

Table 5.9a and 5.9b show the IAE results of variables that affect to separation section for the change in the step increase of quencher outlet temperature in HDA process and the IAE results of all control variables for the disturbance loads of methane mole fraction in fresh feed gas in HDA process respectively.

For the change in the step increase of quencher outlet temperature can be seen that the IAE results for SET1 look just the same as SET2, but IAE results for SET3 are larger than SET2 in all control structure.

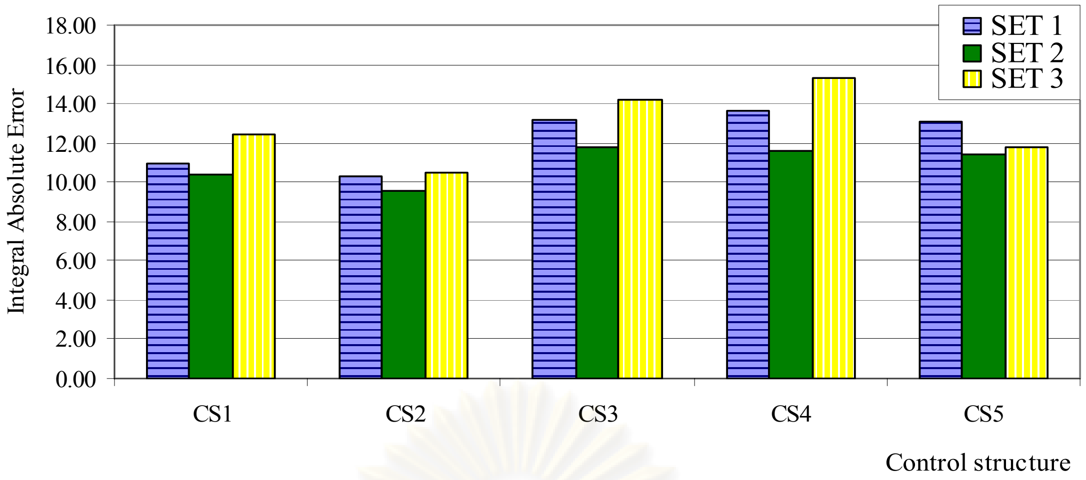


**Figure 5.4** The IAE results of considerate controlled variables to a change the methane mole fraction in fresh feed gas.

**Table 5.9a** The IAE results of variables that affect to separation section for CS1-CS5 to a change in quencher outlet temperature.

| | SET 1 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| LIQ-Temp | 0.977 | 0.976 | 1.022 | 1.023 | 1.021 |
| LIQ-P | 0.017 | 0.019 | 0.029 | 0.018 | 0.014 |
| LIQ-FLOW | 0.989 | 0.989 | 1.007 | 1.007 | 1.008 |
| LIQ - Comp Mole Frac (Benzene) | 1.444 | 1.434 | 1.169 | 1.175 | 1.094 |
| LIQ - Comp Mole Frac (BiPhenyl) | 1.498 | 1.493 | 1.198 | 1.199 | 1.127 |
| LIQ - Comp Mole Frac (Hydrogen) | 0.434 | 0.459 | 0.362 | 0.345 | 0.364 |
| LIQ - Comp Mole Frac (Methane) | 0.272 | 0.274 | 0.219 | 0.222 | 0.218 |
| LIQ - Comp Mole Frac (Toluene) | 1.461 | 1.453 | 1.178 | 1.184 | 1.105 |
| SUM | 7.092 | 7.099 | 6.183 | 6.173 | 5.951 |

| | SET 2 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| LIQ-Temp | 0.976 | 0.976 | 1.022 | 1.023 | 1.016 |
| LIQ-P | 0.014 | 0.020 | 0.023 | 0.015 | 0.016 |
| LIQ-FLOW | 0.989 | 0.989 | 1.008 | 1.008 | 1.008 |
| LIQ - Comp Mole Frac (Benzene) | 1.385 | 1.377 | 1.064 | 1.075 | 1.047 |
| LIQ - Comp Mole Frac (BiPhenyl) | 1.440 | 1.437 | 1.106 | 1.107 | 1.093 |
| LIQ - Comp Mole Frac (Hydrogen) | 0.557 | 0.583 | 0.453 | 0.438 | 0.467 |
| LIQ - Comp Mole Frac (Methane) | 0.173 | 0.178 | 0.148 | 0.149 | 0.150 |
| LIQ - Comp Mole Frac (Toluene) | 1.407 | 1.400 | 1.080 | 1.089 | 1.064 |
| SUM | 6.941 | 6.959 | 5.905 | 5.903 | 5.860 |

| SET 3 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| LIQ-Temp | 0.960 | 0.960 | 1.019 | 1.019 | 1.011 |
| LIQ-P | 2.683 | 2.670 | 3.156 | 3.181 | 3.126 |
| LIQ-FLOW | 0.981 | 0.982 | 1.012 | 1.012 | 1.011 |
| LIQ - Comp Mole Frac (Benzene) | 1.075 | 1.094 | 0.211 | 0.216 | 0.142 |
| LIQ - Comp Mole Frac (BiPhenyl) | 0.926 | 0.954 | 0.183 | 0.189 | 0.050 |
| LIQ - Comp Mole Frac (Hydrogen) | 2.137 | 2.112 | 2.115 | 2.111 | 2.064 |
| LIQ - Comp Mole Frac (Methane) | 2.382 | 2.439 | 2.700 | 2.720 | 2.755 |
| LIQ - Comp Mole Frac (Toluene) | 0.914 | 0.929 | 0.288 | 0.294 | 0.152 |
| SUM | 12.057 | 12.139 | 10.685 | 10.742 | 10.311 |

**Table 5.9b** The IAE results of variables that affect to separation section for CS1-CS5 to a change in methane mole fraction of fresh feed gas.

| SET 1 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| LIQ-Temp | 0.509 | 0.316 | 1.487 | 1.667 | 1.325 |
| LIQ-P | 0.532 | 0.615 | 0.564 | 0.528 | 0.616 |
| LIQ-FLOW | 2.120 | 2.009 | 0.397 | 0.406 | 0.355 |
| LIQ - Comp Mole Frac (Benzene) | 1.122 | 1.044 | 1.072 | 1.119 | 0.967 |
| LIQ - Comp Mole Frac (BiPhenyl) | 1.095 | 0.996 | 1.079 | 1.144 | 0.989 |
| LIQ - Comp Mole Frac (Hydrogen) | 1.168 | 0.877 | 0.998 | 1.031 | 0.792 |
| LIQ - Comp Mole Frac (Methane) | 0.950 | 1.103 | 1.067 | 0.947 | 1.071 |
| LIQ - Comp Mole Frac (Toluene) | 1.116 | 1.023 | 1.067 | 1.126 | 0.962 |
| SUM | 8.611 | 7.983 | 7.731 | 7.969 | 7.078 |

| SET 2 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| LIQ-Temp | 0.458 | 0.240 | 1.289 | 1.385 | 1.159 |
| LIQ-P | 0.529 | 0.597 | 0.485 | 0.525 | 0.592 |
| LIQ-FLOW | 2.018 | 1.914 | 0.327 | 0.332 | 0.310 |
| LIQ - Comp Mole Frac (Benzene) | 1.130 | 1.059 | 0.856 | 0.887 | 0.760 |
| LIQ - Comp Mole Frac (BiPhenyl) | 1.102 | 1.012 | 0.861 | 0.914 | 0.778 |
| LIQ - Comp Mole Frac (Hydrogen) | 1.031 | 0.756 | 1.111 | 1.117 | 0.896 |
| LIQ - Comp Mole Frac (Methane) | 0.973 | 1.135 | 1.022 | 0.908 | 1.052 |
| LIQ - Comp Mole Frac (Toluene) | 1.124 | 1.038 | 0.853 | 0.897 | 0.757 |
| SUM | 8.365 | 7.751 | 6.803 | 6.964 | 6.304 |

| SET 3 | | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| LIQ-Temp | 0.559 | 0.220 | 1.461 | 1.792 | 1.133 |
| LIQ-P | 2.706 | 2.454 | 1.276 | 1.959 | 1.023 |
| LIQ-FLOW | 1.974 | 1.804 | 0.351 | 0.380 | 0.302 |
| LIQ - Comp Mole Frac (Benzene) | 1.180 | 1.079 | 0.947 | 1.014 | 0.764 |
| LIQ - Comp Mole Frac (BiPhenyl) | 1.193 | 1.054 | 0.961 | 1.036 | 0.786 |
| LIQ - Comp Mole Frac (Hydrogen) | 1.216 | 0.764 | 1.168 | 1.235 | 0.839 |
| LIQ - Comp Mole Frac (Methane) | 0.776 | 1.173 | 0.988 | 0.679 | 1.156 |
| LIQ - Comp Mole Frac (Toluene) | 1.207 | 1.075 | 0.954 | 1.038 | 0.763 |
| SUM | 10.811 | 9.623 | 8.107 | 9.133 | 6.766 |

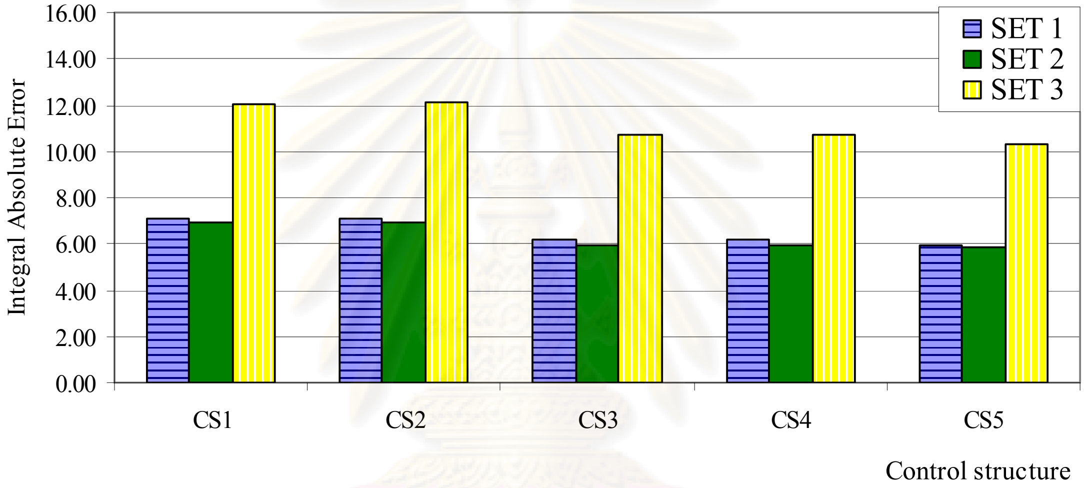


**Figure 5.5** The IAE results of variables that affect to separation section to a change the quencher outlet temperature.

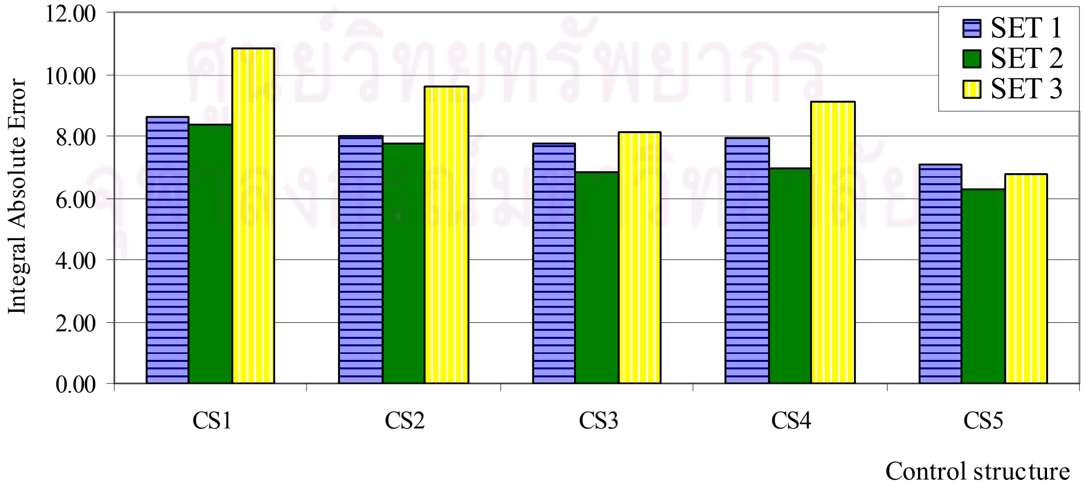


**Figure 5.6** The IAE results of variables that affect to separation section to a change the methane mole fractions in fresh feed gas.

Figure 5.5 and 5.6 show the affect to separation section for the change in the step increase of quencher outlet temperature in HDA process and the IAE results of all control variables for the disturbance loads of methane mole fraction in fresh feed gas in HDA process respectively.

As can be seen that the controlled variables of SET2 have the most effective, the IAE results of variables in separator liquid stream are smaller than SET1 and SET3 so the disturbance propagation to separation section are small on compared with the other.

### 5.2.2 Comparison our control structure with REF1 and REF2 reference.

Table 5.10a and 5.10b show the IAE results for change in the disturbance of quencher outlet temperature and methane mole fraction in fresh feed gas respectively.

As can be seen that when disturbance occurring our control structures (CS1-CS5) are the most effective on compared with REF1 on every set (SET1-SET3). The IAE results of our control structure (CS1-CS5) in every set are the same with REF2.

**Table 5.10a** The IAE results of the control loop for each set to a change in quencher outlet temperature compare with REF1 and REF2.

| | SET1 | | | | | | |
|---|---|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 | REF1 | REF2 |
| Tquench | 0.989 | 0.979 | 0.983 | 1.000 | 0.996 | 1.066 | 0.989 |
| Trin | 0.333 | 0.321 | 0.333 | 0.331 | 0.330 | 5.036 | 0.317 |
| Psep | 0.897 | 0.981 | 1.471 | 0.918 | 0.720 | - | 1.187 |
| rH2 | 0.106 | 0.053 | 0.395 | 0.238 | 0.161 | 5.083 | - |
| Xmet,sep vap | 0.810 | 0.889 | 1.231 | 1.261 | 0.809 | - | - |
| Xmet,GREC | - | - | - | - | - | - | 1.000 |
| FFH2 | 0.703 | 0.157 | 0.565 | 0.713 | 0.148 | 3.972 | - |
| FFTOL | 0.157 | 0.143 | 1.984 | 1.009 | 0.764 | 1.956 | - |
| TSEP | 1.111 | 1.110 | 1.160 | 1.161 | 1.159 | 0.194 | 1.121 |
| Xmet,mix | - | - | - | - | - | 3.322 | - |
| Prin | - | - | - | - | - | 1.767 | - |
| Xtol,quench | - | - | - | - | - | 1.000 | - |
| Ftottol | - | - | - | - | - | - | 1.000 |
| **SUM** | **5.106** | **4.634** | **8.122** | **6.631** | **5.087** | **23.396** | **5.614** |

| | SET2 | | | | | | |
|---|---|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 | REF1 | REF2 |
| Tquench | 0.987 | 0.979 | 0.979 | 0.999 | 0.998 | 1.066 | 0.989 |
| Trin | 0.334 | 0.321 | 0.340 | 0.324 | 0.330 | 5.036 | 0.317 |
| Psep | 0.712 | 1.001 | 1.188 | 0.752 | 0.800 | - | 1.187 |
| rH2 | 0.092 | 0.048 | 0.320 | 0.203 | 0.144 | 5.083 | - |
| Xmet,sep vap | - | - | - | - | - | - | - |
| Xmet,GREC | - | - | - | - | - | - | 1.000 |
| FFH2 | 0.660 | 0.162 | 0.540 | 0.677 | 0.158 | 3.972 | - |
| FFTOL | 0.147 | 0.140 | 1.923 | 0.892 | 0.714 | 1.956 | - |
| TSEP | 1.108 | 1.109 | 1.162 | 1.161 | 1.163 | 0.194 | 1.121 |
| Xmet,mix | 0.213 | 0.147 | 0.222 | 0.295 | 0.127 | 3.322 | - |
| Prin | - | - | - | - | - | 1.767 | - |
| Xtol,quench | - | - | - | - | - | 1.000 | - |
| Ftottol | - | - | - | - | - | - | 1.000 |
| **SUM** | **4.253** | **3.907** | **6.673** | **5.304** | **4.435** | **23.396** | **5.614** |

| | SET3 | | | | | | |
|---|---|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 | REF1 | REF2 |
| Tquench | 0.984 | 0.977 | 0.981 | 1.007 | 0.999 | 1.066 | 0.989 |
| Trin | 0.320 | 0.314 | 0.335 | 0.349 | 0.328 | 5.036 | 0.317 |
| Psep | - | - | - | - | - | - | 1.187 |
| rH2 | 0.106 | 0.047 | 0.302 | 0.381 | 0.156 | 5.083 | - |
| Xmet,sep vap | - | - | - | - | - | - | - |
| Xmet,GREC | - | - | - | - | - | - | 1.000 |
| FFH2 | 0.285 | 0.183 | 0.633 | 0.345 | 0.154 | 3.972 | - |
| FFTOL | 0.148 | 0.144 | 1.879 | 1.122 | 0.967 | 1.956 | - |
| TSEP | 1.091 | 1.091 | 1.160 | 1.159 | 1.149 | 0.194 | 1.121 |
| Xmet,mix | 0.364 | 0.172 | 0.722 | 0.714 | 0.058 | 3.322 | - |
| Prin | 0.389 | 0.441 | 0.943 | 0.523 | 0.401 | 1.767 | - |
| Xtol,quench | - | - | - | - | - | 1.000 | - |
| Ftottol | - | - | - | - | - | - | 1.000 |
| **SUM** | **3.686** | **3.369** | **6.954** | **5.599** | **4.211** | **23.396** | **5.614** |

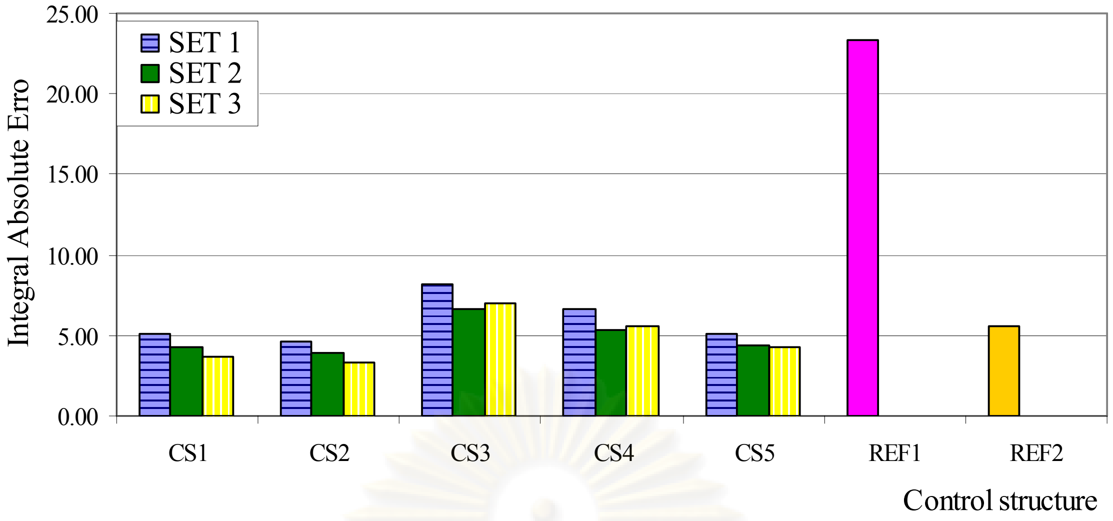


**Figure 5.7** The IAE results of control loop to a change the quencher outlet temperature.

**Table 5.10b** The IAE results of the control loop for each set to a change in methane mole fraction of fresh feed gas compare with REF1 and REF2.

| | SET1 | | | | | | |
|---|---|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 | REF1 | REF2 |
| Tquench | 0.969 | 0.700 | 0.934 | 0.971 | 0.748 | 2.669 | 0.265 |
| Trin | 0.040 | 0.041 | 0.263 | 0.327 | 0.267 | 6.074 | 0.053 |
| Psep | 0.698 | 0.808 | 0.740 | 0.693 | 0.808 | - | 1.891 |
| rH2 | 0.121 | 0.099 | 0.227 | 0.403 | 0.284 | 4.923 | - |
| Xmet,sep vap | 1.052 | 0.934 | 1.054 | 1.046 | 0.914 | - | - |
| Xmet,GREC | - | - | - | - | - | - | 1.000 |
| FFH2 | 0.198 | 0.195 | 0.230 | 0.228 | 0.262 | 4.861 | - |
| FFTOL | 0.092 | 0.056 | 1.544 | 1.237 | 1.659 | 1.906 | - |
| TSEP | 0.603 | 0.382 | 1.898 | 2.127 | 1.683 | 0.483 | 0.202 |
| Xmet,mix | - | - | - | - | - | 1.773 | - |
| Prin | - | - | - | - | - | 1.215 | - |
| Xtol,quench | - | - | - | - | - | 1.000 | - |
| Ftottol | - | - | - | - | - | - | 1.000 |
| SUM | 3.772 | 3.215 | 6.891 | 7.034 | 6.626 | 24.905 | 4.410 |

SET2

| | CS1 | CS2 | CS3 | CS4 | CS5 | REF1 | REF2 |
|---|---|---|---|---|---|---|---|
| Tquench | 0.845 | 0.581 | 0.869 | 0.792 | 0.626 | 2.669 | 0.265 |
| Trin | 0.038 | 0.020 | 0.232 | 0.269 | 0.221 | 6.074 | 0.053 |
| Psep | 0.695 | 0.784 | 0.636 | 0.689 | 0.777 | 0.000 | 1.891 |
| rH2 | 0.103 | 0.081 | 0.224 | 0.328 | 0.235 | 4.923 | - |
| Xmet,sep vap | - | - | - | - | - | - | - |
| Xmet,GREC | - | - | - | - | - | - | 1.000 |
| FFH2 | 0.195 | 0.194 | 0.222 | 0.216 | 0.251 | 4.861 | - |
| FFTOL | 0.079 | 0.032 | 1.366 | 0.993 | 1.392 | 1.906 | - |
| TSEP | 0.544 | 0.288 | 1.651 | 1.768 | 1.456 | 0.483 | 0.202 |
| Xmet,mix | 0.799 | 0.709 | 0.795 | 0.793 | 0.699 | 1.773 | - |
| Prin | - | - | - | - | - | 1.215 | - |
| Xtol,quench | - | - | - | - | - | 1.000 | - |
| Ftottol | - | - | - | - | - | - | 1.000 |
| **SUM** | **3.298** | **2.688** | **5.996** | **5.846** | **5.658** | **24.905** | **4.410** |

SET3

| | CS1 | CS2 | CS3 | CS4 | CS5 | REF1 | REF2 |
|---|---|---|---|---|---|---|---|
| Tquench | 0.963 | 0.515 | 0.953 | 1.109 | 0.622 | 2.669 | 0.265 |
| Trin | 0.053 | 0.026 | 0.247 | 0.352 | 0.220 | 6.074 | 0.053 |
| Psep | - | - | - | - | - | - | 1.891 |
| rH2 | 0.116 | 0.076 | 0.228 | 0.483 | 0.225 | 4.923 | - |
| Xmet,sep vap | - | - | - | - | - | - | - |
| Xmet,GREC | - | - | - | - | - | - | 1.000 |
| FFH2 | 0.193 | 0.193 | 0.381 | 0.201 | 0.257 | 4.861 | - |
| FFTOL | 0.105 | 0.036 | 1.522 | 0.679 | 1.488 | 1.906 | - |
| TSEP | 0.667 | 0.272 | 1.871 | 2.298 | 1.438 | 0.483 | 0.202 |
| Xmet,mix | 0.806 | 0.708 | 0.858 | 0.822 | 0.693 | 1.773 | - |
| Prin | 0.820 | 0.937 | 0.865 | 0.822 | 0.911 | 1.215 | - |
| Xtol,quench | - | - | - | - | - | 1.000 | - |
| Ftottol | - | - | - | - | - | - | 1.000 |
| **SUM** | **3.723** | **2.762** | **6.925** | **6.766** | **5.854** | **24.905** | **4.410** |

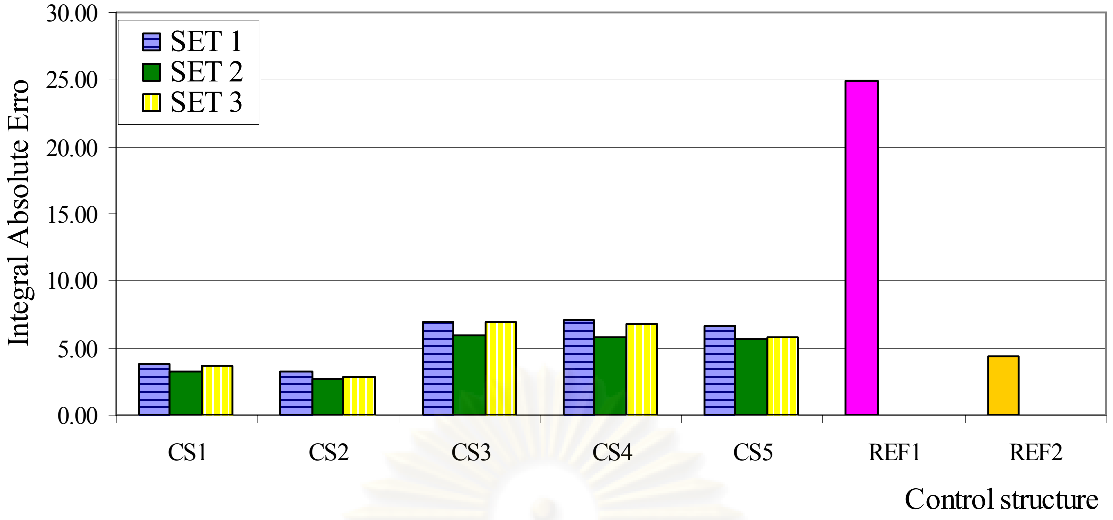


**Figure 5.8** The IAE results of control loop to a change the methane mole fraction in fresh feed gas.

### 5.2.3 Economic analysis for decision the set of controlled variable.

This section evaluates economics of a HDA process. The term economics refers to the evaluation of the operating costs associated with the operation of a HDA process. The methods consider the continuing costs associated with the daily operation of the process and the benefit obtained from benzene product are combined into meaningful economic criteria are provided.

In this work, we evaluate economic of each control structure by using benzene product and operational (energy) cost when disturbance occurs. Two dynamic disturbances used to evaluate operational cost in 10 hours. The economic results are shown compare with steady-state value.

Table 5.11 and 5.12 show the utility usage compare with steady-state value of a change in the disturbance loads of quencher outlet temperature and methane mole fraction in fresh feed gas respectively.

Table 5.13 and 5.14 show the operating cost (product – raw material) compare with steady-state value of a change in the disturbance loads of quencher outlet temperature and methane mole fraction in fresh feed gas respectively. The negative value means save cost on compared with steady-state value. The negative value or lower positive value is the better.

As can be seen that the high profit are control structure 1 (CS1) of SET1 for quencher outlet temperature disturbance and control structure 1 (CS1) of SET3 for methane mole fraction load disturbance on compared with structure is fixed work of compressor.

Comparison between structure that the work of compressor is used (Ws = manipulated variable), can be seen that control structure 5 (CS5) of SET3 given the most profit for disturbance of quencher outlet temperature and control structure 5 of SET2 given the most profit for disturbance of methane mole fraction in fresh feed gas.

Table 5.11 The utility usage compare with steady-state value of a change in quencher outlet temperature.

| UTILITY USAGE - DIVIATION FROM SS - SET1 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | lbmole | | MBtu | | (hp) | MBtu | | | | | | lbmole |
| CS | FFTOL | FFH2 | Qfur | Qcooler | Ws | QC1 | QR1 | QC2 | QR2 | QC3 | QR3 | Benzene Product |
| CS1 | 4104.37 | 4262.23 | -29002.44 | -28932.36 | 0.00 | -8.39 | 75.56 | 249.76 | 13.90 | 100.54 | 41.13 | 5299.62 |
| CS2 | 4418.86 | 4107.35 | -29001.89 | -28933.09 | 0.00 | -8.36 | 79.86 | 249.42 | 10.18 | 100.49 | 40.77 | 5292.02 |
| CS3 | 17.50 | -1396.51 | -29654.45 | -29693.75 | -16755.74 | -5.35 | 26.36 | 81.84 | -2.91 | 54.54 | 25.69 | 1720.94 |
| CS4 | 18.00 | -1458.49 | -29660.05 | -29698.84 | -16881.10 | -5.32 | 28.26 | 79.90 | -6.57 | 53.39 | 26.20 | 1685.44 |
| CS5 | 18.40 | -1948.70 | -29693.19 | -29746.10 | -18411.47 | -4.79 | 20.89 | 64.06 | -5.60 | 75.47 | 24.25 | 1368.17 |

| UTILITY USAGE - DIVIATION FROM SS - SET2 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | lbmole | | MBtu | | (hp) | MBtu | | | | | | lbmole |
| CS | FFTOL | FFH2 | Qfur | Qcooler | Ws | QC1 | QR1 | QC2 | QR2 | QC3 | QR3 | Benzene Product |
| CS1 | 5013.62 | 5660.32 | -28993.46 | -28912.60 | 0.00 | -8.52 | 81.43 | 270.38 | 14.73 | 99.36 | 40.67 | 5842.27 |
| CS2 | 5168.06 | 5650.50 | -28993.23 | -28913.71 | 0.00 | -8.54 | 82.70 | 273.02 | 14.87 | 108.65 | 41.63 | 5821.30 |
| CS3 | 18.31 | -847.10 | -29713.29 | -29753.57 | -18462.42 | -5.18 | 25.79 | 81.45 | -4.97 | 54.38 | 24.80 | 1829.89 |
| CS4 | 19.04 | -893.44 | -29718.84 | -29761.88 | -18652.05 | -5.16 | 27.73 | 87.66 | -5.99 | 52.46 | 25.09 | 1822.42 |
| CS5 | 19.02 | -734.75 | -29704.99 | -29742.81 | -18106.07 | -5.38 | 26.39 | 88.86 | 1.90 | 55.85 | 26.01 | 1878.92 |

| UTILITY USAGE - DIVIATION FROM SS - SET3 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | lbmole | | MBtu | | (hp) | MBtu | | | | | | lbmole |
| CS | FFTOL | FFH2 | Qfur | Qcooler | Ws | QC1 | QR1 | QC2 | QR2 | QC3 | QR3 | Benzene Product |
| CS1 | 11383.16 | 15287.13 | -28626.37 | -28446.04 | 0.00 | -20.34 | 124.28 | 514.71 | 58.56 | 82.75 | 40.44 | 11070.59 |
| CS2 | 10959.75 | 14212.94 | -28630.47 | -28459.32 | 0.00 | -20.03 | 120.05 | 493.89 | 59.58 | 86.39 | 40.03 | 10621.50 |
| CS3 | -18.90 | 296.20 | -29982.41 | -30103.39 | -48739.50 | -11.55 | -11.41 | 76.09 | 15.10 | -12.55 | -4.45 | 1606.96 |
| CS4 | -18.97 | 308.14 | -29981.01 | -30103.16 | -48823.63 | -11.60 | -6.34 | 74.21 | 16.76 | -12.33 | -4.74 | 1601.65 |
| CS5 | -19.54 | 196.42 | -29903.12 | -30009.68 | -44971.76 | -12.35 | -8.31 | 87.55 | 13.54 | 3.60 | 0.38 | 1795.04 |

(+) utility usage or product increase from steady-state

(-) utility usage or product decrease from steady-state

Table 5.12 The utility usage compare with steady-state value of a change in methane mole fraction of fresh feed gas.

UTILITY USAGE - DIVIATION FROM SS - SET1

| | lbmole | | MBtu | | (hp) | MBtu | | | | | | lbmole |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CS | FFTOL | FFH2 | Qfur | Qcooler | Ws | QC1 | QR1 | QC2 | QR2 | QC3 | QR3 | Benzene Product |
| CS1 | 24854.04 | 1232774.24 | 2624.90 | 3003.93 | 0.00 | -24.07 | 206.03 | 542.87 | 23.39 | 272.54 | 98.69 | -10819.42 |
| CS2 | 28854.10 | 1239525.90 | 2741.41 | 3172.98 | 0.00 | -27.21 | 237.20 | 681.09 | 44.58 | 259.50 | 97.43 | -14001.51 |
| CS3 | 29.78 | 1210703.21 | 246.84 | 33.44 | -99820.69 | 0.54 | -61.31 | -329.04 | -62.94 | 97.72 | 28.64 | 11202.29 |
| CS4 | 28.27 | 1210709.15 | 436.18 | 257.93 | -89471.35 | 0.06 | -47.40 | -317.88 | -70.94 | 125.07 | 40.08 | 14239.39 |
| CS5 | 28.50 | 1211619.78 | 130.26 | -109.22 | -106896.31 | 1.25 | -73.35 | -352.30 | -59.95 | 134.42 | 15.70 | -7014.25 |

UTILITY USAGE - DIVIATION FROM SS - SET2

| | lbmole | | MBtu | | (hp) | MBtu | | | | | | lbmole |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CS | FFTOL | FFH2 | Qfur | Qcooler | Ws | QC1 | QR1 | QC2 | QR2 | QC3 | QR3 | Benzene Product |
| CS1 | 24488.83 | 1229145.87 | 2615.41 | 2985.10 | 0.00 | -23.25 | 202.56 | 520.43 | 16.84 | 274.01 | 98.28 | 10882.44 |
| CS2 | 28205.33 | 1235268.94 | 2730.01 | 3146.84 | 0.00 | -26.36 | 228.42 | 649.84 | 39.27 | 286.14 | 98.64 | 13647.70 |
| CS3 | 20.05 | 1207798.73 | 417.61 | 215.90 | -92339.19 | -0.65 | -56.26 | -333.06 | -71.49 | 110.95 | 33.43 | -7074.24 |
| CS4 | 20.02 | 1208244.01 | 540.11 | 362.74 | -85076.82 | -0.49 | -46.33 | -322.86 | -76.35 | 129.80 | 41.33 | -6848.90 |
| CS5 | 18.27 | 1209116.69 | 302.60 | 80.56 | -99398.30 | -0.15 | -67.36 | -343.19 | -60.75 | 87.37 | 24.04 | -7235.34 |

UTILITY USAGE - DIVIATION FROM SS - SET3

| | lbmole | | MBtu | | (hp) | MBtu | | | | | | lbmole |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CS | FFTOL | FFH2 | Qfur | Qcooler | Ws | QC1 | QR1 | QC2 | QR2 | QC3 | QR3 | Benzene Product |
| CS1 | 21421.05 | 1225146.64 | 2426.07 | 2748.74 | 0.00 | -18.95 | 179.05 | 407.11 | -2.20 | 281.28 | 99.46 | 8436.21 |
| CS2 | 26833.98 | 1233942.18 | 2638.04 | 3035.71 | 0.00 | -24.58 | 215.25 | 598.59 | 36.21 | 263.51 | 98.04 | 12643.79 |
| CS3 | 14.02 | 1208110.39 | 449.61 | 262.22 | -89566.67 | -0.40 | -51.72 | -326.27 | -73.45 | 122.08 | 37.40 | -6962.61 |
| CS4 | 12.79 | 1208663.05 | 621.88 | 473.08 | -77879.80 | 0.44 | -31.07 | -314.16 | -77.13 | 155.42 | 50.41 | -6627.94 |
| CS5 | 8.02 | 1208868.42 | 264.55 | 30.67 | -102462.04 | -0.42 | -73.85 | -354.93 | -66.50 | 148.13 | 18.41 | -7501.53 |

(+) utility usage or product increase from steady-state

(-) utility usage or product decrease from steady-state

**Table 5.13** The operating profit compare with steady-state value of a change in quencher outlet temperature.

| | COST ($) - SET1 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| FFTOL | 24790.39 | 26689.94 | 105.70 | 108.72 | 111.14 |
| FFH2 | 4858.94 | 4682.37 | -1592.02 | -1662.68 | -2221.51 |
| Qfur | -116009.78 | -116007.57 | -118617.81 | -118640.20 | -118772.76 |
| Qcooler | -677.02 | -677.03 | -694.83 | -694.95 | -696.06 |
| Ws | 0.00 | 0.00 | -703.74 | -709.01 | -773.28 |
| QC1 | -0.20 | -0.20 | -0.13 | -0.12 | -0.11 |
| QR1 | 188.89 | 199.66 | 65.90 | 70.65 | 52.22 |
| QC2 | 5.84 | 5.84 | 1.92 | 1.87 | 1.50 |
| QR2 | 34.74 | 25.46 | -7.26 | -16.42 | -14.00 |
| QC3 | 2.35 | 2.35 | 1.28 | 1.25 | 1.77 |
| QR3 | 102.84 | 101.92 | 64.23 | 65.50 | 60.61 |
| Benzene Product | 47908.52 | 47839.82 | 15557.25 | 15236.38 | 12368.21 |
| SUM Cost ($) | -134611.51 | -132817.07 | -136934.02 | -136711.78 | -134618.70 |

| | COST ($) – SET2 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| FFTOL | 30282.26 | 31215.08 | 110.62 | 115.00 | 114.85 |
| FFH2 | 6452.76 | 6441.57 | -965.70 | -1018.52 | -837.61 |
| Qfur | -115973.83 | -115972.90 | -118853.17 | -118875.36 | -118819.95 |
| Qcooler | -676.55 | -676.58 | -696.23 | -696.43 | -695.98 |
| Ws | 0.00 | 0.00 | -775.42 | -783.39 | -760.45 |
| QC1 | -0.20 | -0.20 | -0.12 | -0.12 | -0.13 |
| QR1 | 203.57 | 206.75 | 64.47 | 69.33 | 65.99 |
| QC2 | 6.33 | 6.39 | 1.91 | 2.05 | 2.08 |
| QR2 | 36.81 | 37.17 | -12.42 | -14.98 | 4.74 |
| QC3 | 2.33 | 2.54 | 1.27 | 1.23 | 1.31 |
| QR3 | 101.68 | 104.07 | 61.99 | 62.73 | 65.02 |
| Benzene Product | 52814.17 | 52624.60 | 16542.21 | 16474.68 | 16985.44 |
| SUM Cost ($) | -132379.02 | -131260.71 | -137605.01 | -137613.14 | -137845.57 |

| | COST ($) – SET3 | | | | |
|---|---|---|---|---|---|
| | CS1 | CS2 | CS3 | CS4 | CS5 |
| FFTOL | 68754.29 | 66196.92 | -114.13 | -114.55 | -118.02 |
| FFH2 | 17427.33 | 16202.75 | 337.67 | 351.28 | 223.92 |
| Qfur | -114505.50 | -114521.88 | -119929.62 | -119924.03 | -119612.48 |
| Qcooler | -665.64 | -665.95 | -704.42 | -704.41 | -702.23 |
| Ws | 0.00 | 0.00 | -2047.06 | -2050.59 | -1888.81 |
| QC1 | -0.48 | -0.47 | -0.27 | -0.27 | -0.29 |
| QR1 | 310.69 | 300.12 | -28.52 | -15.85 | -20.78 |
| QC2 | 12.04 | 11.56 | 1.78 | 1.74 | 2.05 |
| QR2 | 146.41 | 148.94 | 37.74 | 41.89 | 33.85 |
| QC3 | 1.94 | 2.02 | -0.29 | -0.29 | 0.08 |
| QR3 | 101.10 | 100.09 | -11.11 | -11.84 | 0.96 |
| Benzene Product | 100078.18 | 96018.41 | 14526.87 | 14478.92 | 16227.12 |
| SUM Cost ($) | -128495.99 | -128244.30 | -136985.10 | -136905.85 | -138308.87 |

(+) higher operating cost from steady-state

(-) lower operating cost from steady-state (high profit)

**Table 5.14** The operating profit compare with steady-state value of a change in methane mole fraction of fresh feed gas.

COST ($) - SET1

| | CS1 | CS2 | CS3 | CS4 | CS5 |
|---|---|---|---|---|---|
| FFTOL | 150118.43 | 174278.76 | 179.87 | 170.78 | 172.17 |
| FFH2 | 1405362.63 | 1413059.53 | 1380201.65 | 1380208.43 | 1381246.55 |
| Qfur | 10499.59 | 10965.66 | 987.37 | 1744.72 | 521.02 |
| Qcooler | 70.29 | 74.25 | 0.78 | 6.04 | -2.56 |
| Ws | 0.00 | 0.00 | -4192.47 | -3757.80 | -4489.65 |
| QC1 | -0.56 | -0.64 | 0.01 | 0.00 | 0.03 |
| QR1 | 515.09 | 593.01 | -153.27 | -118.49 | -183.38 |
| QC2 | 12.70 | 15.94 | -7.70 | -7.44 | -8.24 |
| QR2 | 58.46 | 111.44 | -157.36 | -177.36 | -149.88 |
| QC3 | 6.38 | 6.07 | 2.29 | 2.93 | 3.15 |
| QR3 | 246.72 | 243.58 | 71.61 | 100.20 | 39.25 |
| Benzene Product | 101268.70 | 128724.09 | -63408.82 | -60748.30 | -66653.82 |
| SUM Cost ($) | 1465621.03 | 1470623.51 | 1440341.62 | 1438920.30 | 1443802.28 |

COST ($) – SET2

| | CS1 | CS2 | CS3 | CS4 | CS5 |
|---|---|---|---|---|---|
| FFTOL | 147912.50 | 170360.19 | 121.10 | 120.95 | 110.38 |
| FFH2 | 1401226.29 | 1408206.59 | 1376890.55 | 1377398.17 | 1378393.02 |
| Qfur | 10461.66 | 10920.02 | 1670.46 | 2160.45 | 1210.41 |
| Qcooler | 69.85 | 73.64 | 5.05 | 8.49 | 1.89 |
| Ws | 0.00 | 0.00 | -3878.25 | -3573.23 | -4174.73 |
| QC1 | -0.54 | -0.62 | -0.02 | -0.01 | 0.00 |
| QR1 | 506.41 | 571.05 | -140.65 | -115.82 | -168.40 |
| QC2 | 12.18 | 15.21 | -7.79 | -7.56 | -8.03 |
| QR2 | 42.09 | 98.19 | -178.73 | -190.86 | -151.88 |
| QC3 | 6.41 | 6.70 | 2.60 | 3.04 | 2.04 |
| QR3 | 245.70 | 246.60 | 83.57 | 103.33 | 60.09 |
| Benzene Product | 98377.30 | 123375.16 | -63951.17 | -61914.06 | -65407.47 |
| SUM Cost ($) | 1462105.24 | 1467122.41 | 1438519.06 | 1437821.00 | 1440682.26 |

COST ($) – SET3

| | CS1 | CS2 | CS3 | CS4 | CS5 |
|---|---|---|---|---|---|
| FFTOL | 129383.17 | 162077.21 | 84.68 | 77.28 | 48.44 |
| FFH2 | 1396667.17 | 1406694.08 | 1377245.84 | 1377875.88 | 1378110.00 |
| Qfur | 9704.26 | 10552.17 | 1798.43 | 2487.53 | 1058.18 |
| Qcooler | 64.32 | 71.04 | 6.14 | 11.07 | 0.72 |
| Ws | 0.00 | 0.00 | -3761.80 | -3270.95 | -4303.41 |
| QC1 | -0.44 | -0.58 | -0.01 | 0.01 | -0.01 |
| QR1 | 447.64 | 538.12 | -129.30 | -77.66 | -184.62 |
| QC2 | 9.53 | 14.01 | -7.63 | -7.35 | -8.31 |
| QR2 | -5.50 | 90.52 | -183.62 | -192.81 | -166.24 |
| QC3 | 6.58 | 6.17 | 2.86 | 3.64 | 3.47 |
| QR3 | 248.64 | 245.09 | 93.51 | 126.02 | 46.03 |
| Benzene Product | 76263.29 | 114299.86 | -62941.99 | -59916.62 | -67813.88 |
| SUM Cost ($) | 1460262.07 | 1465987.96 | 1438091.09 | 1436949.27 | 1442418.14 |

(+) higher operating cost from steady-state

(-) lower operating cost from steady-state (high profit)

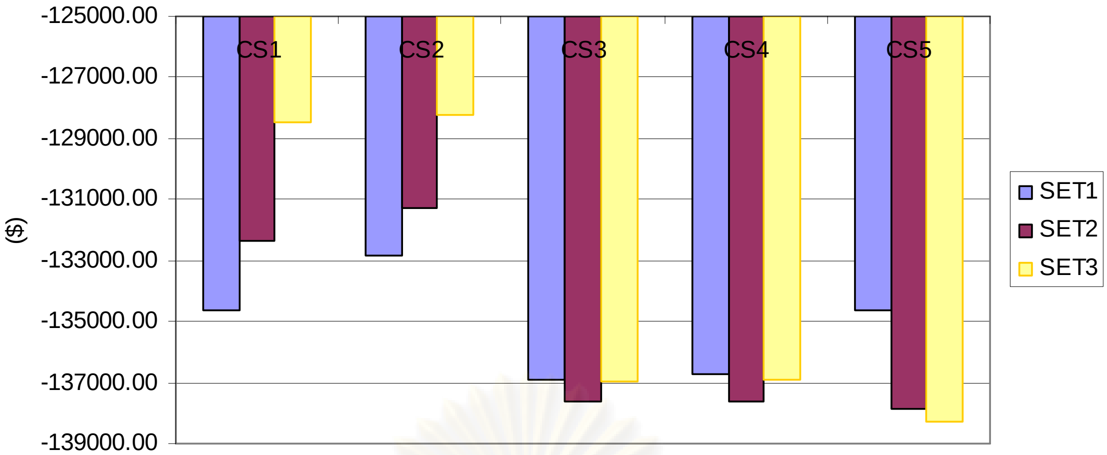


**Figure 5.9** The operating profit compare with steady-state value for a change in quencher outlet temperature.

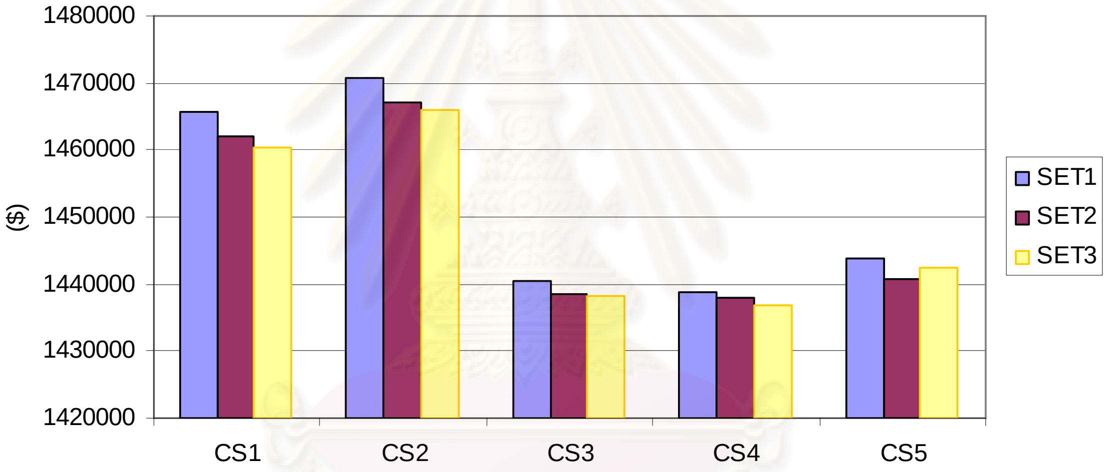


**Figure 5.10** The operating profit compare with steady-state value for a change in methane mole fraction of fresh feed gas.

From above we can conclude that

1. If we consider only the performance of control loop, SET1-SET3 gives the same performance.
2. If we consider the performance of control loop plus other variables (include difference variables in every set (SET1-SET3)), the SET2 gives the most effective because a little disturbance propagate to other point (small IAE at the points are not controlled) and the next is SET1.

3. If we consider the disturbance propagate to separation section, SET1 and SET2 gives the same smaller disturbance propagate to separation section.
4. Control structure 2 (CS2) and Control structure 5 (CS5) are the best structure for all set of controlled variables.
5. If we consider the cost value when disturbance occur, SET3 (CS4) gives the small cost on compared with other.

As conclusions above we can see that

1. The fixture point theorem to bring the best set of controlled variable. Why we say that although SET1 does not give the best response on compared with SET2, because SET1 and SET2 are the same controlled variables but difference methane mole fraction position control. Methane mole fraction in SET2 is near the manipulated so the IAE value is smaller than SET1. Therefore we can say that the fixture point given the best set of controlled variables.
2. The best control configurations depend on the direction of controlled variable with manipulated variable.

### 5.2.4 Economic analysis of this work compare with REF1 and REF2.

Table 5.15 and 5.16 show the utility usage of reference control structure REF1 and REF2 compare with steady-state value for a change in the disturbance loads of quencher outlet temperature and methane mole fraction in fresh feed gas respectively.

Table 5.17 and 5.18 show the operating cost (product – raw material) compare with steady-state value for a change in the disturbance loads of quencher outlet temperature and methane mole fraction in fresh feed gas respectively. The negative value means save cost on compared with steady-state value. The negative value or lower positive value is the better.

As Figure 5.11 the operating cost of control structure CS1-CS5 for set of controlled variables SET1-SET3 compare with reference REF1 and REF2 when change in quencher outlet temperature, the operating cost of this work are smaller than the REF1 and similar to REF2.

As Figure 5.12 the operating cost of control structure CS1-CS5 for set of controlled variables SET1-SET3 compare with reference REF1 and REF2 when change in methane mole fraction of fresh feed gas, the operating cost of control structure CS3-CS5 are smaller than the REF1 and REF2.

**Table 5.15** The utility usage of REF1 and REF2 compare with steady-state value of a change in quencher outlet temperature.

| UTILITY USAGE - DIVIATION FROM SS | | | |
|---|---|---|---|
| | | REF1 | REF2 |
| FFTOL | lbmole | -69.56 | -3199.12 |
| FFH2 | lbmole | -36689.76 | -6445.55 |
| Qfur | MBtu | -30757.48 | -29132.83 |
| Qcooler | MBtu | -31051.47 | -29174.96 |
| Ws | hp | 12730.71 | 0.00 |
| QC1 | MBtu | 102.43 | -3.82 |
| QR1 | MBtu | 498.95 | 6.10 |
| QC2 | MBtu | 2769.98 | -27.36 |
| QR2 | MBtu | 2892.67 | -33.31 |
| QC3 | MBtu | 1305.96 | 101.78 |
| QR3 | MBtu | 259.81 | 36.40 |
| Benzene Product | lbmole | -9357.75 | -564.54 |

(+) utility usage or product increase from steady-state

(-) utility usage or product decrease from steady-state

Table 5.16 The operating profit of REF1 and REF2 compare with steady-state value of a change in quencher outlet temperature.

| | Cost ($) | |
|---|---|---|
| | REF1 | REF2 |
| FFTOL | -420.14 | -19322.68 |
| FFH2 | -41826.32 | -7347.92 |
| Qfur | -123029.93 | -116531.31 |
| Qcooler | -726.60 | -682.69 |
| Ws | 534.69 | 0.00 |
| QC1 | 2.40 | -0.09 |
| QR1 | 1247.37 | 15.24 |
| QC2 | 64.82 | -0.64 |
| QR2 | 7231.68 | -83.27 |
| QC3 | 30.56 | 2.38 |
| QR3 | 649.53 | 91.00 |
| Benzene Product | -84594.06 | -5103.40 |
| sum | -71647.90 | -138756.59 |

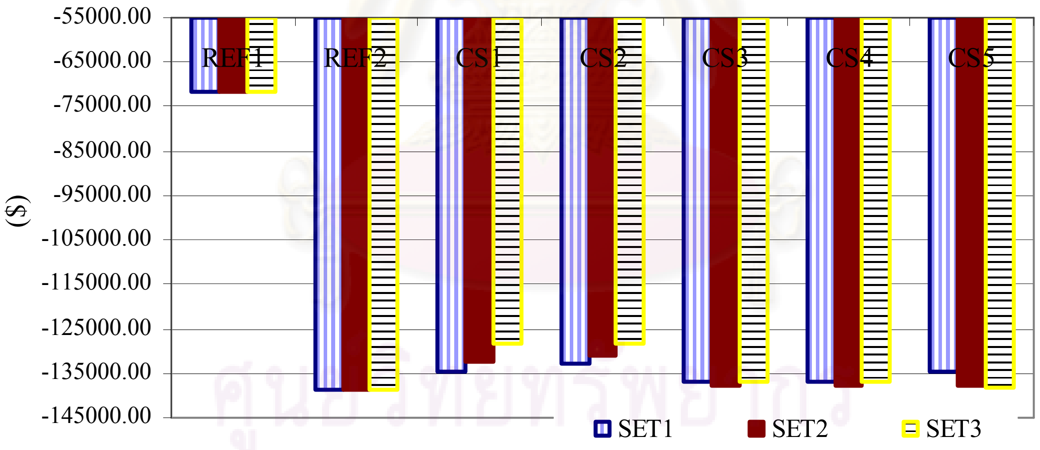


Figure 5.11 The operating profit compare with steady-state value for a change in quencher outlet temperature.

**Table 5.17** The utility usage of REF1 and REF2 compare with steady-state value of a change in methane mole fraction of fresh feed gas.

| UTILITY USAGE - DIVIATION FROM SS | | | |
|---|---|---|---|
| | | REF1 | REF2 |
| FFTOL | lbmole | 11.38 | -8458.00 |
| FFH2 | lbmole | 1196760.36 | 1192976.73 |
| Qfur | MBtu | 1706.93 | 2147.76 |
| Qcooler | MBtu | 1565.71 | 2012.90 |
| Ws | hp | -50519.95 | 0.00 |
| QC1 | MBtu | 2.24 | 3.57 |
| QR1 | MBtu | -67.67 | -88.89 |
| QC2 | MBtu | -629.65 | -668.74 |
| QR2 | MBtu | -146.86 | -175.21 |
| QC3 | MBtu | 12.76 | 277.74 |
| QR3 | MBtu | -28.44 | 79.78 |
| Benzene Product | lbmole | -10819.42 | -14001.51 |

(+) utility usage or product increase from steady-state

(-) utility usage or product decrease from steady-state

**Table 5.18** The operating profit of REF1 and REF2 compare with steady-state value of a change in methane mole fraction of fresh feed gas.

| | Cost ($) | |
|---|---|---|
| | REF1 | REF2 |
| FFTOL | 68.74 | -51086.35 |
| FFH2 | 1364306.81 | 1359993.47 |
| Qfur | 6827.71 | 8591.02 |
| Qcooler | 36.64 | 47.10 |
| Ws | -2121.84 | 0.00 |
| QC1 | 0.05 | 0.08 |
| QR1 | -169.16 | -222.22 |
| QC2 | -14.73 | -15.65 |
| QR2 | -367.14 | -438.02 |
| QC3 | 0.30 | 6.50 |
| QR3 | -71.09 | 199.46 |
| Benzene Product | -97807.51 | -126573.65 |
| sum | 1466303.79 | 1443649.05 |

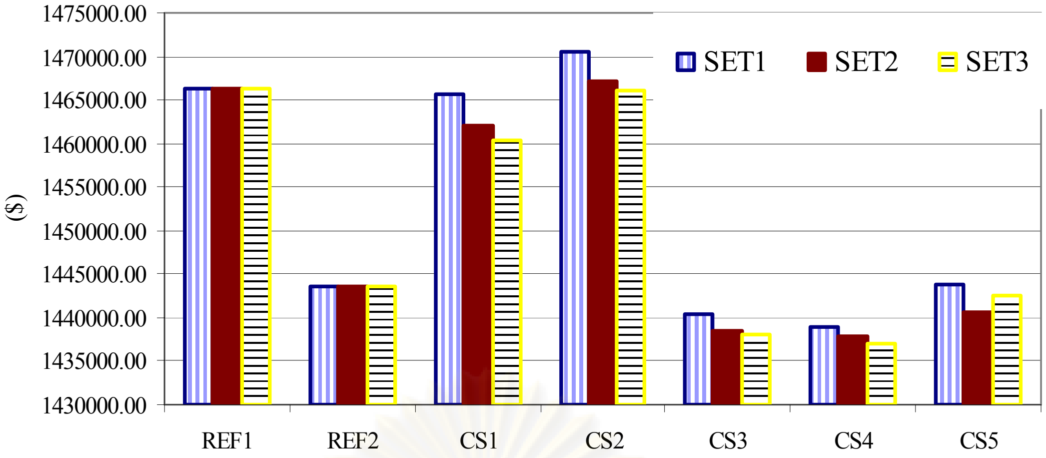


Figure 5.12 The operating profit compare with steady-state value for a change in methane mole fraction of fresh feed gas.

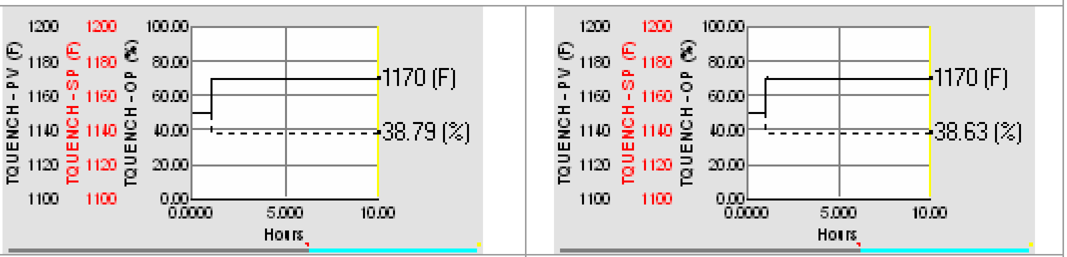
### 5.2.5 Dynamic simulation

This section shows the graph response of dynamic simulation of the SET1 (CS5) and SET2 (CS5) compared with REF1 and REF2.

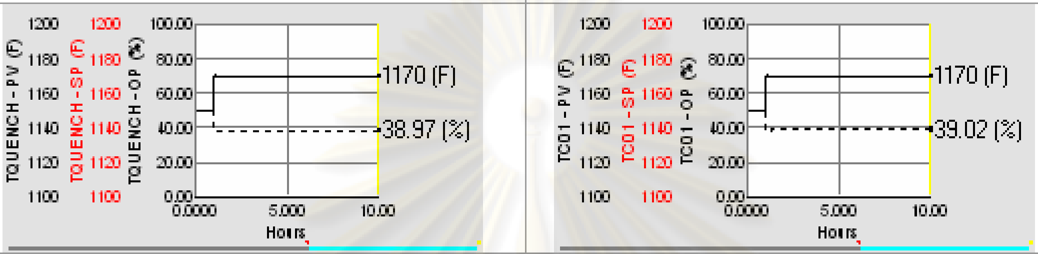
In order to illustrate the dynamic behaviors of our control structures and the previous control structures (Araujo et al., 2006 and Luyben et al., 1998), two types of disturbance are used to test response of the system: quencher outlet temperature step increase 20 °F and methane mole fraction in fresh feed gas increase from 0.03 to 0.08 respectively. The dynamic responses of control structure are shown in Figures 5.13 and Figure 5.14. Note that the disturbances are applied 1 hr after the beginning of each simulation run.

### 5.2.5A Increase in the quencher outlet temperature from 1150 °F to 1170 °F

Quencher outlet temperature



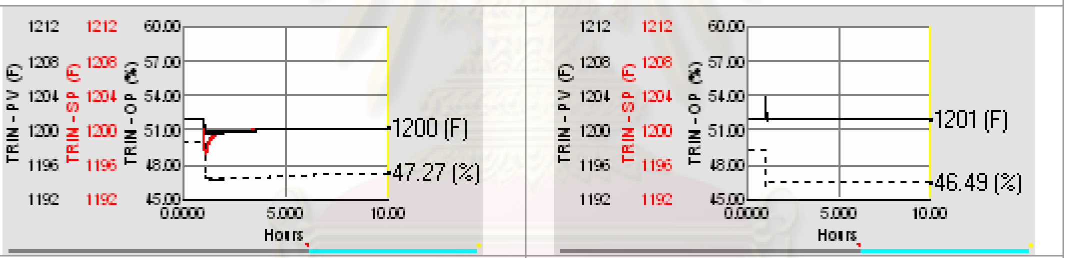
REF1 REF2



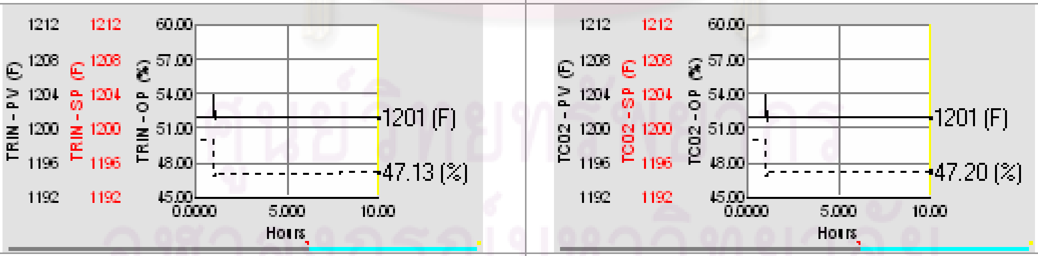
SET1-CS5 SET2-CS5

( A )

Reactor inlet temperature



REF1 REF2

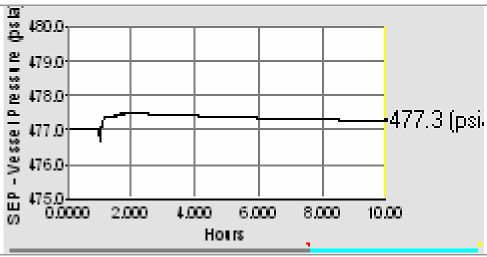


SET1-CS5 SET2-CS5

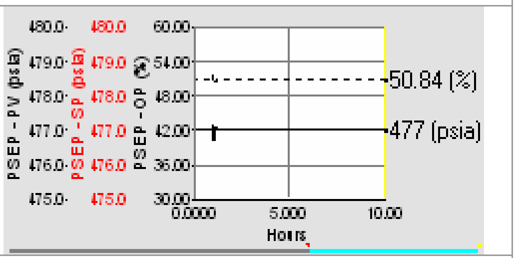
( B )

Figure 5.13 Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

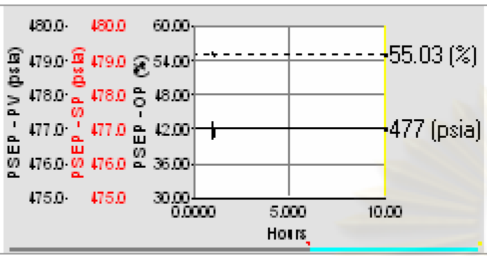
Separator pressure



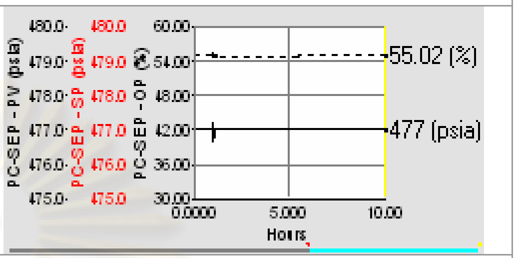
REF1 (Open loop)



REF2



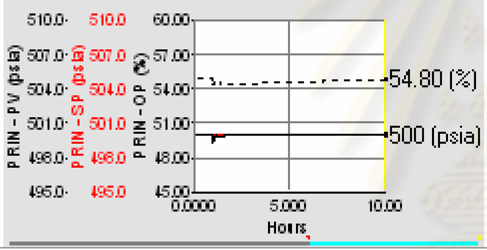
SET1-CS5



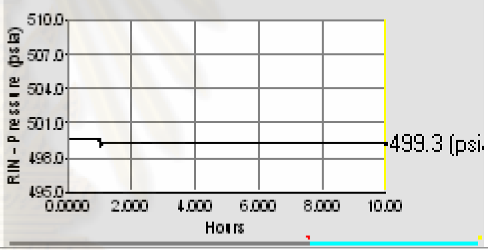
SET2-CS5

( C )

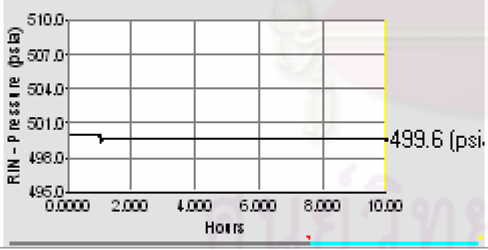
Reactor inlet pressure



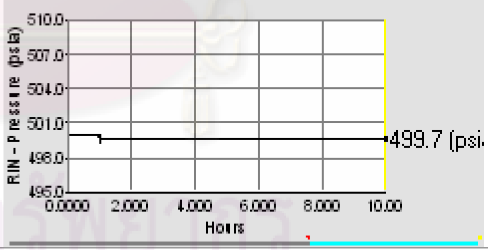
REF1



REF2 (Open loop)



SET1-CS5 (Open loop)



SET2-CS5 (Open loop)

( D )

**Figure 5.13** Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

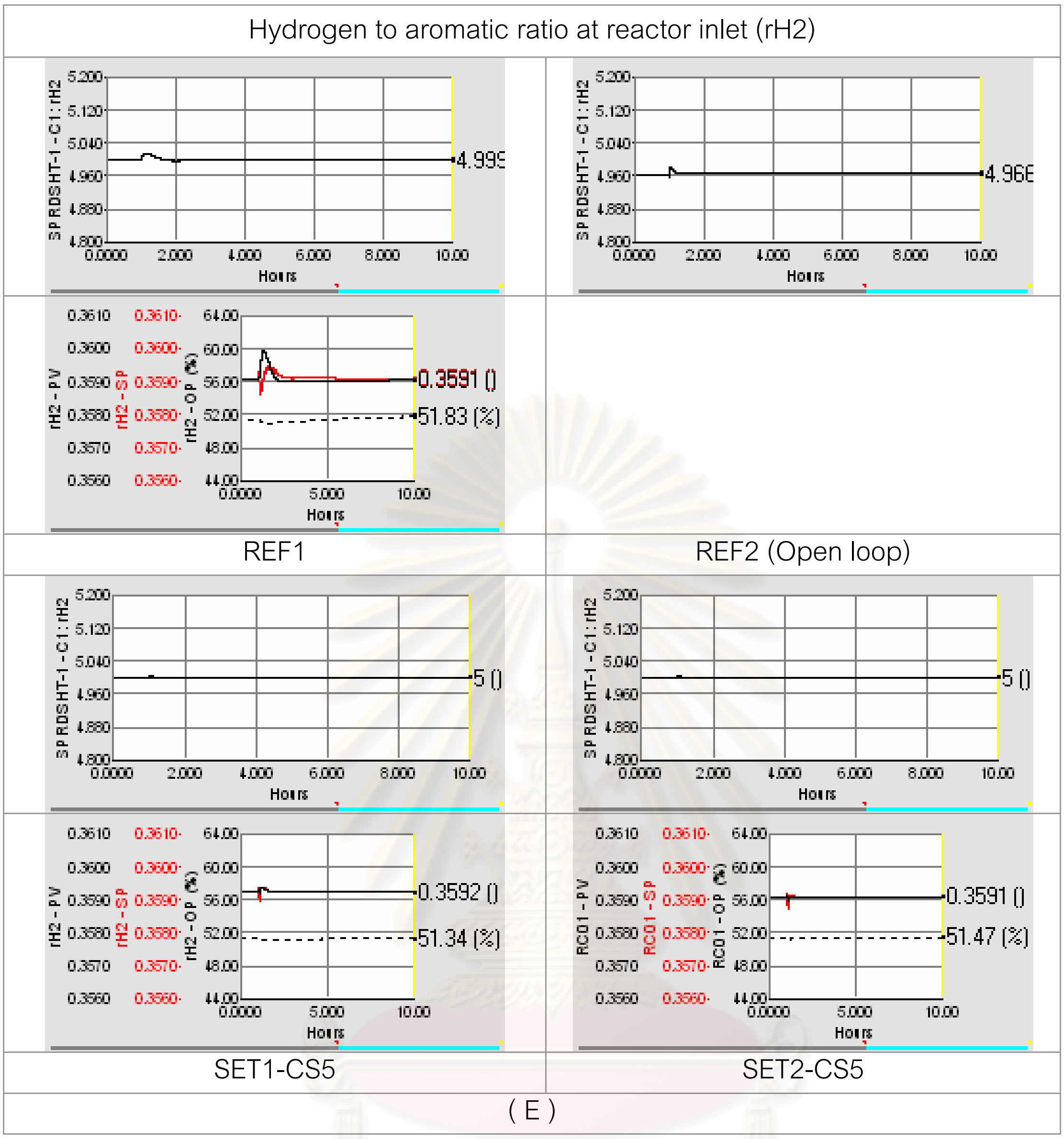
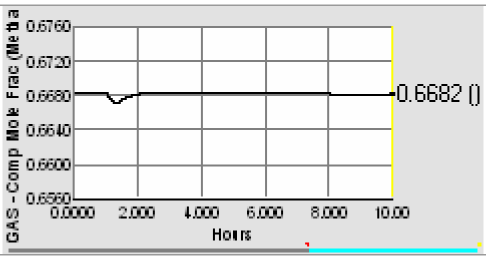


**Figure 5.13** Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

Methane mole fraction on vapor separator stream



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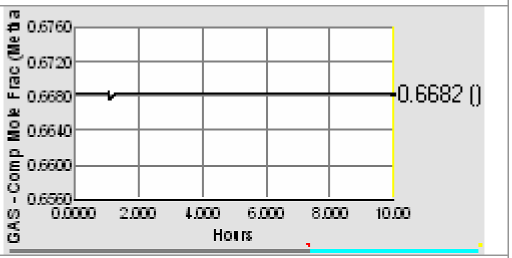

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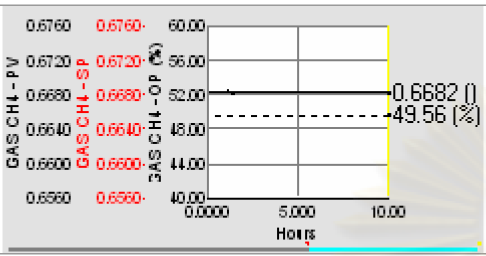
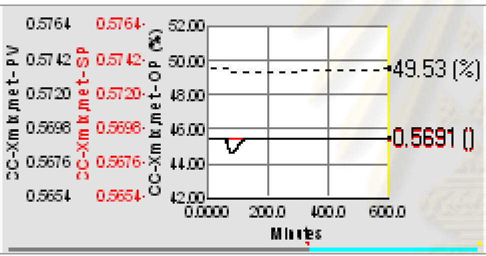


SET1-CS5

SET2-CS5 (Open loop)

( F)

Methane mole fraction on mixture outlet stream



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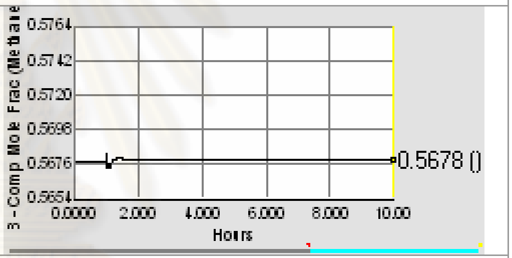

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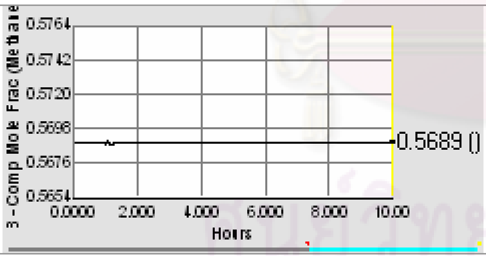
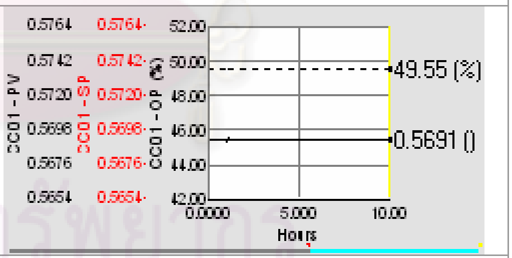


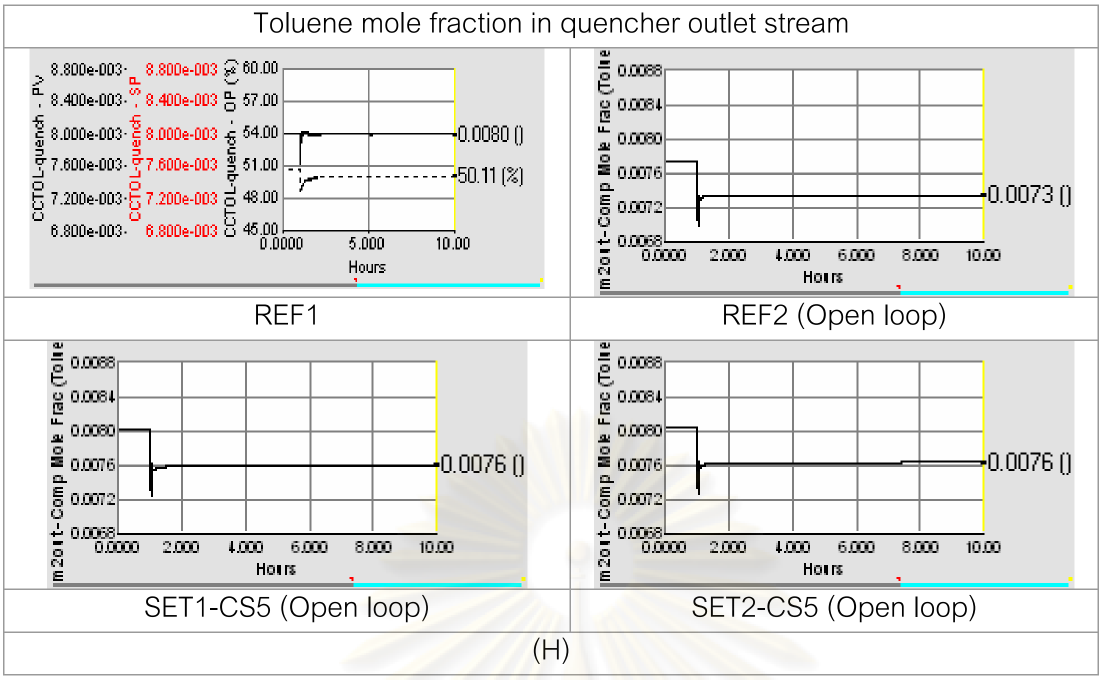
SET1-CS5 (Open loop)



SET2-CS5

(G)

**Figure 5.13** Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product



Toluene mole fraction in quencher outlet stream

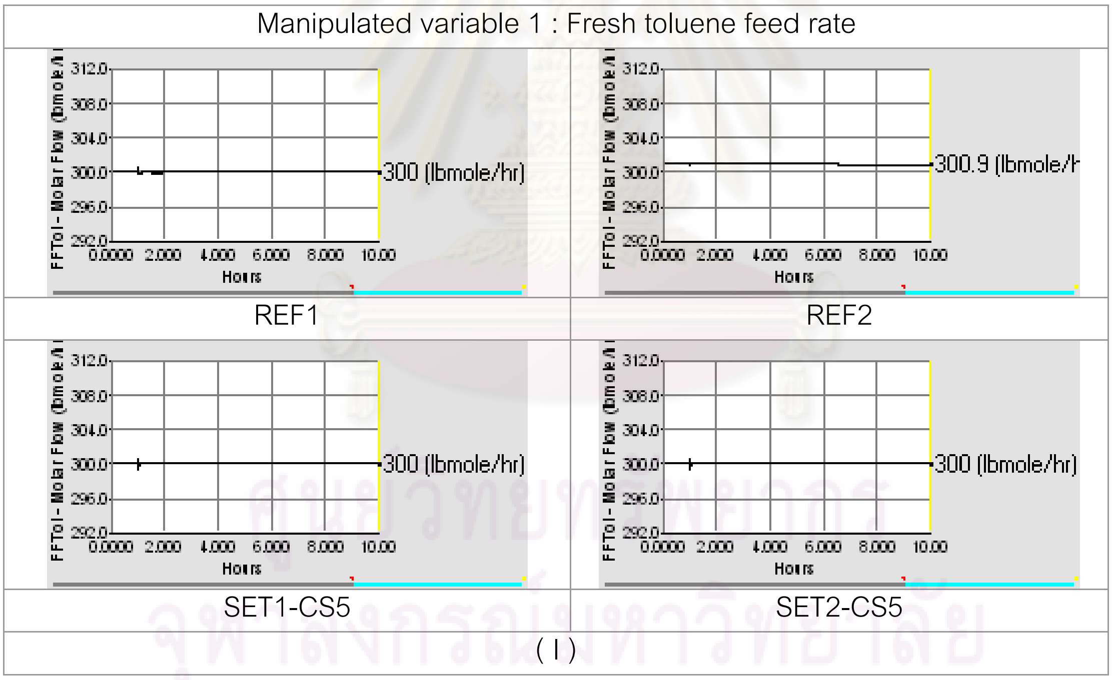
REF1

REF2 (Open loop)

SET1-CS5 (Open loop)

SET2-CS5 (Open loop)

(H)



Manipulated variable 1 : Fresh toluene feed rate

REF1

REF2

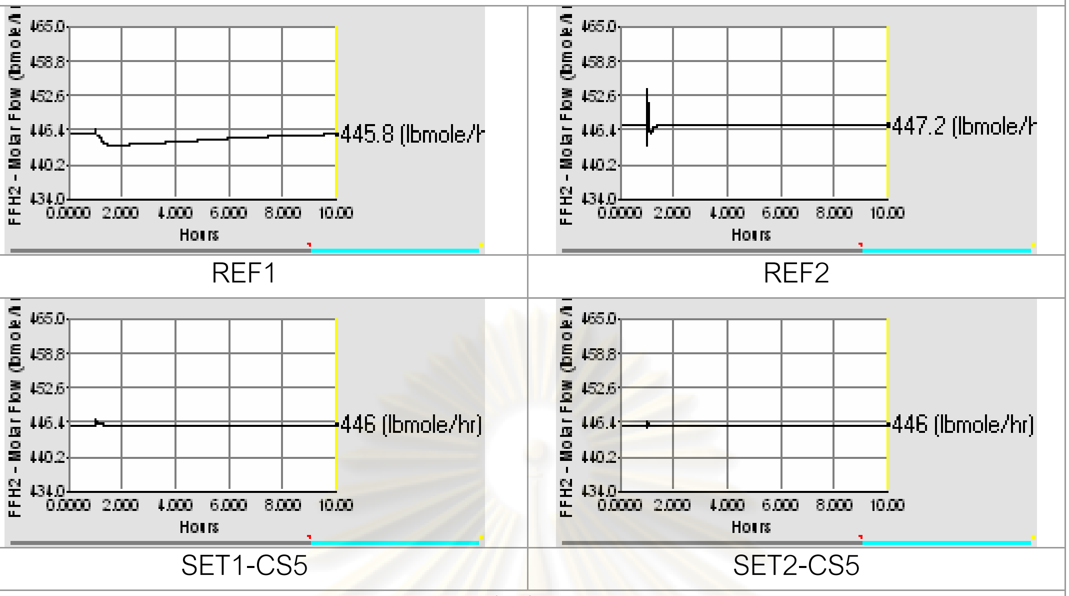
SET1-CS5

SET2-CS5

( I )

**Figure 5.13** Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

Manipulated variable 2 : Fresh gas feed rate

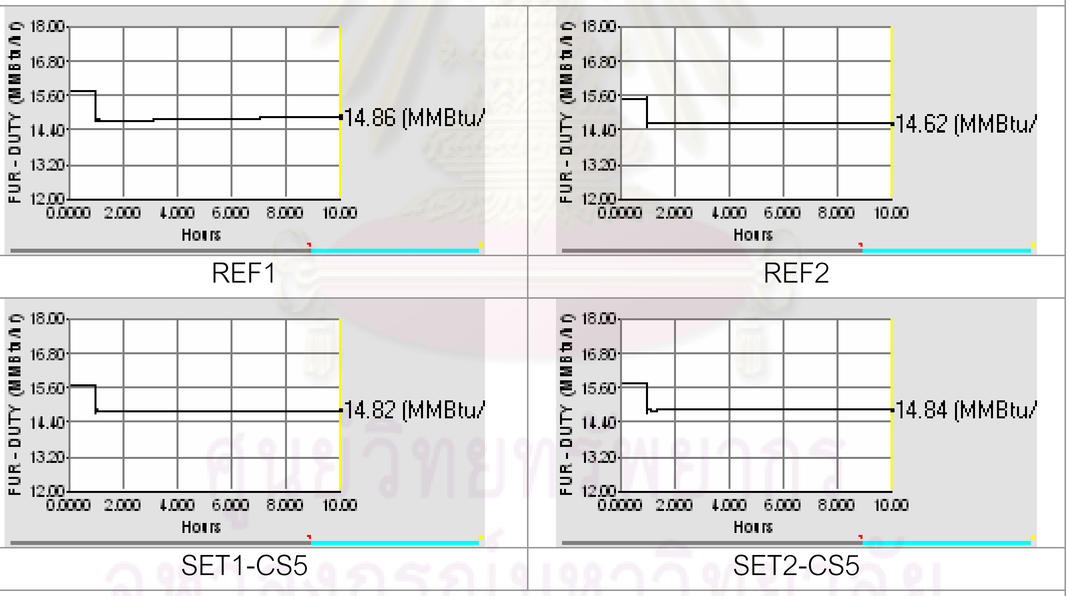


REF1 REF2

SET1-CS5 SET2-CS5

( J )

Manipulated variable 3 : Furnace heat duty

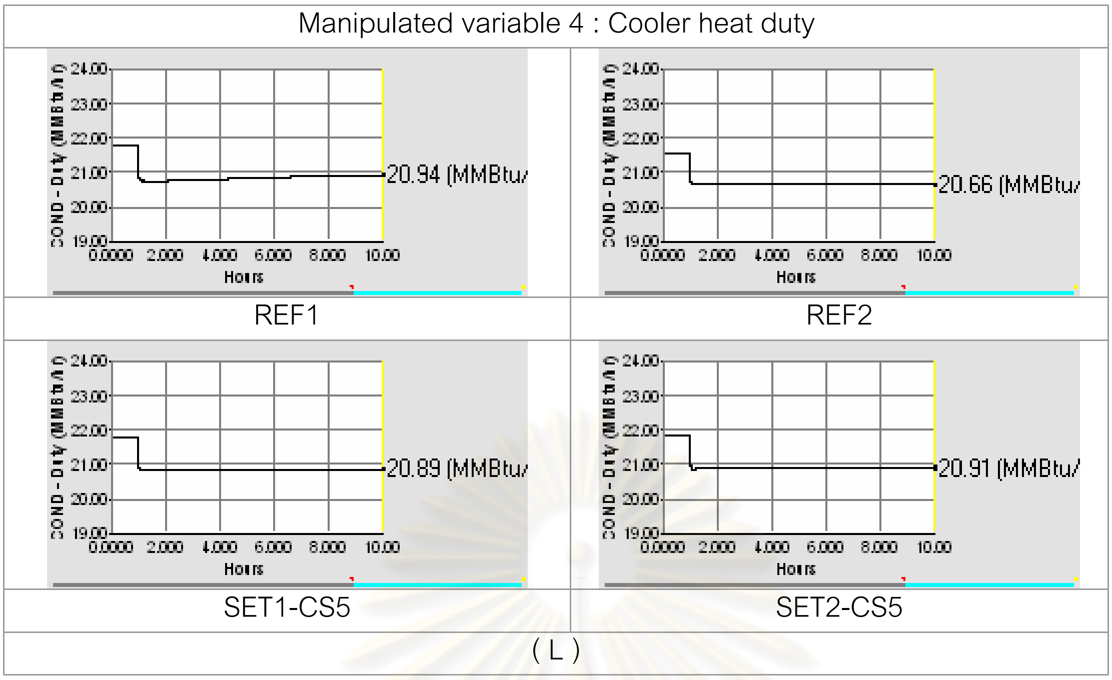


REF1 REF2

SET1-CS5 SET2-CS5

( K )

**Figure 5.13** Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

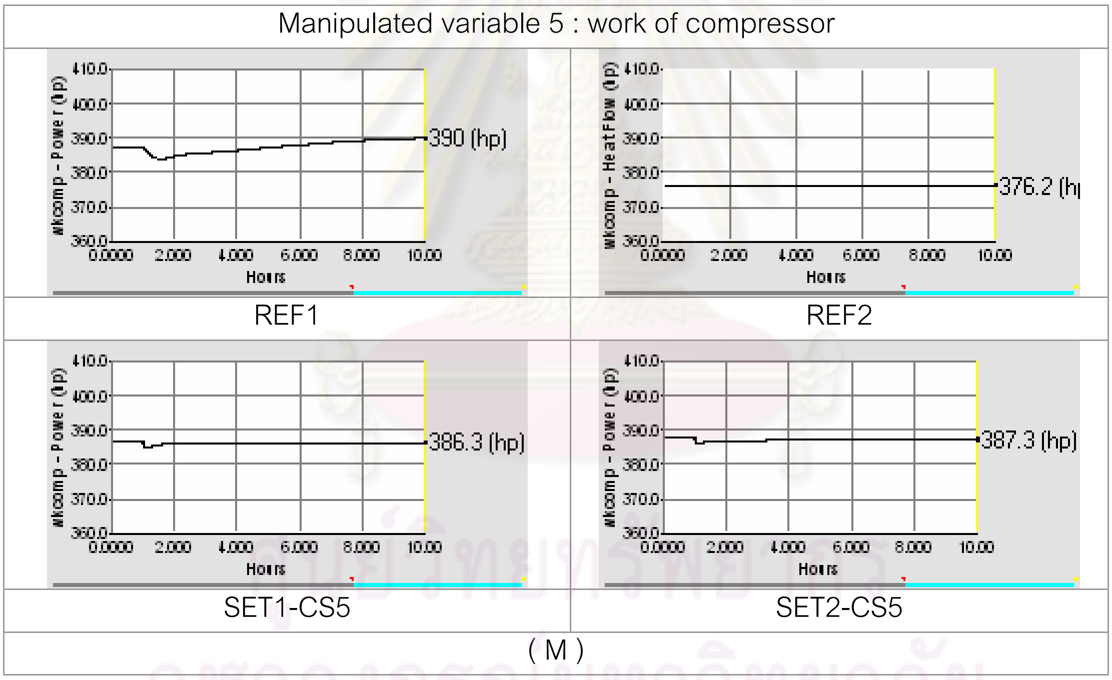


Manipulated variable 4 : Cooler heat duty

REF1 REF2

SET1-CS5 SET2-CS5

( L )



Manipulated variable 5 : work of compressor

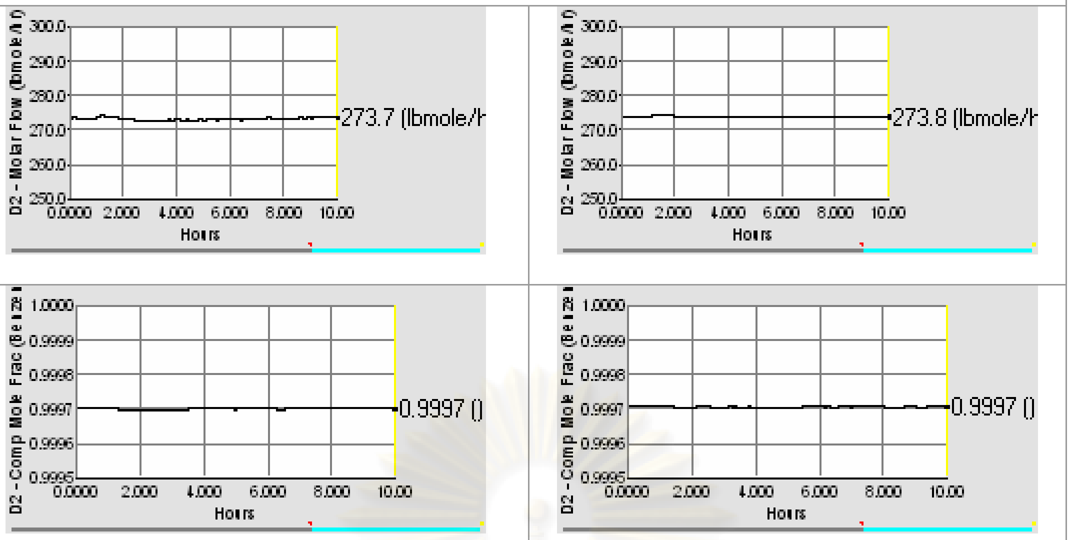
REF1 REF2

SET1-CS5 SET2-CS5

( M )

**Figure 5.13** Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

Benzene product



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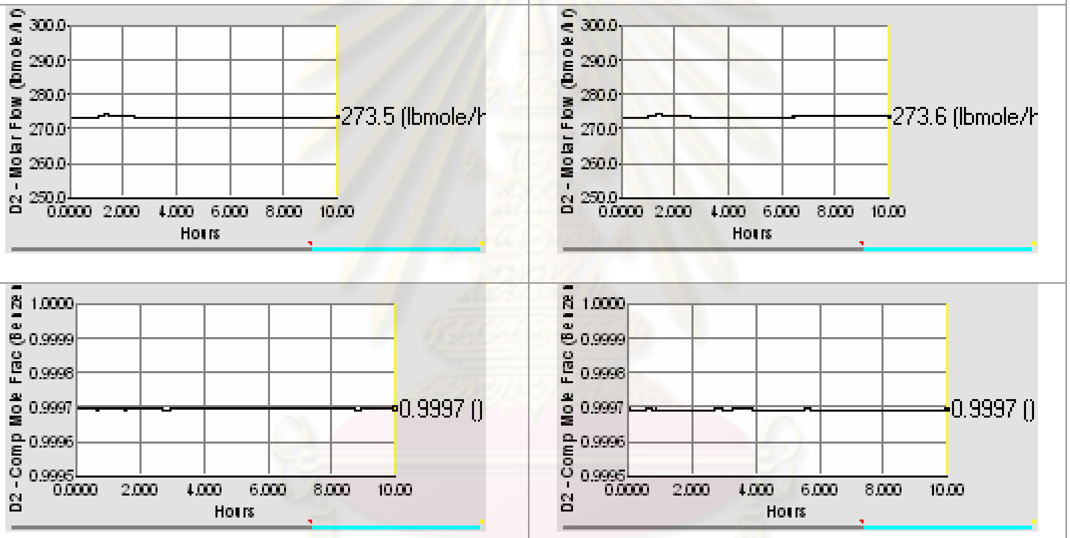


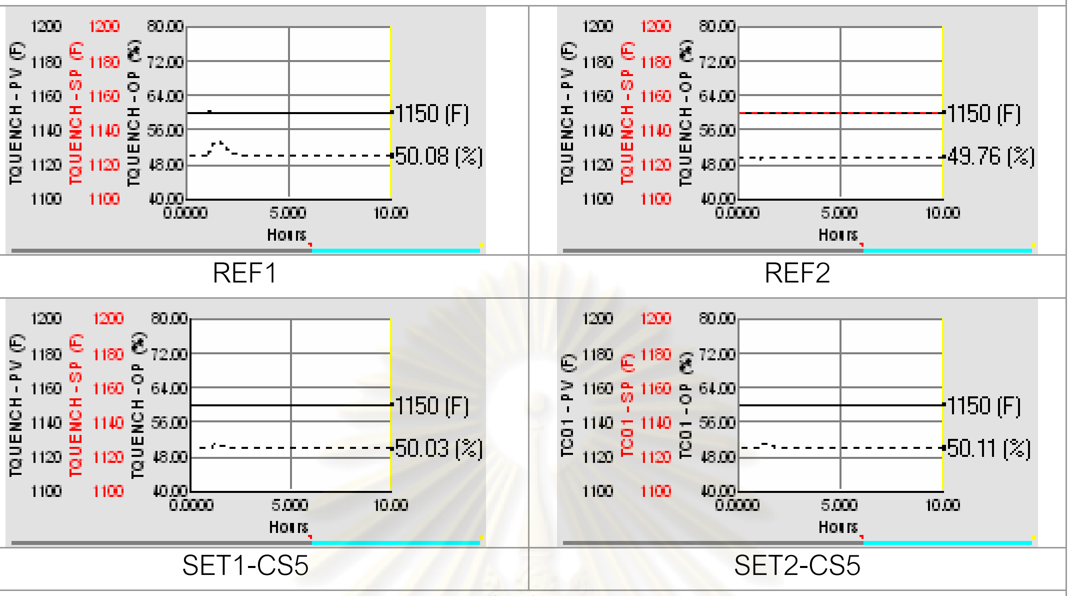
SET1-CS5 SET2-CS5

( N )

**Figure 5.13** Dynamic responses of increase 20 °F in quencher outlet temperature for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

5.2.5B Increase in the methane mole fraction in fresh hydrogen feed from 0.03 to 0.08.

Quencher outlet temperature

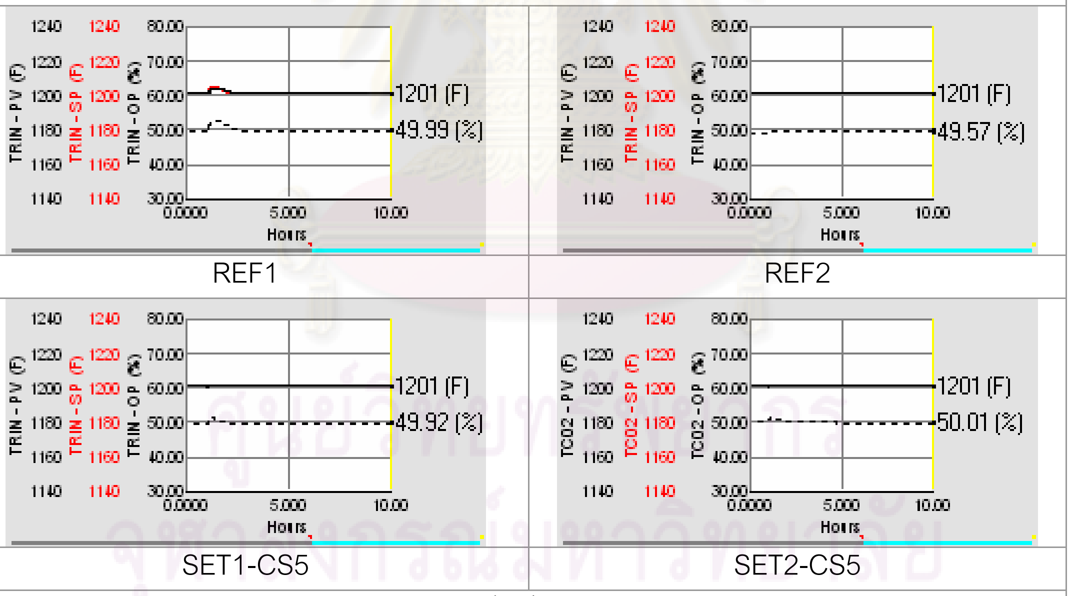


REF1 REF2

SET1-CS5 SET2-CS5

( A )

Reactor inlet temperature

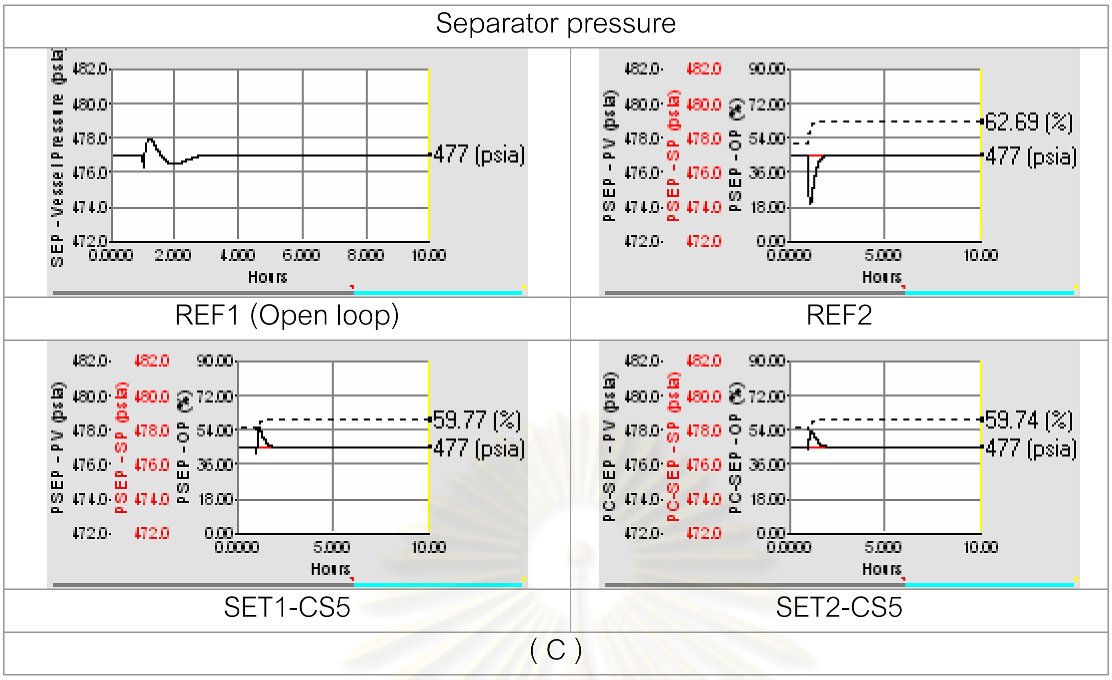


REF1 REF2

SET1-CS5 SET2-CS5

( B )

**Figure 5.14** Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product



Separator pressure

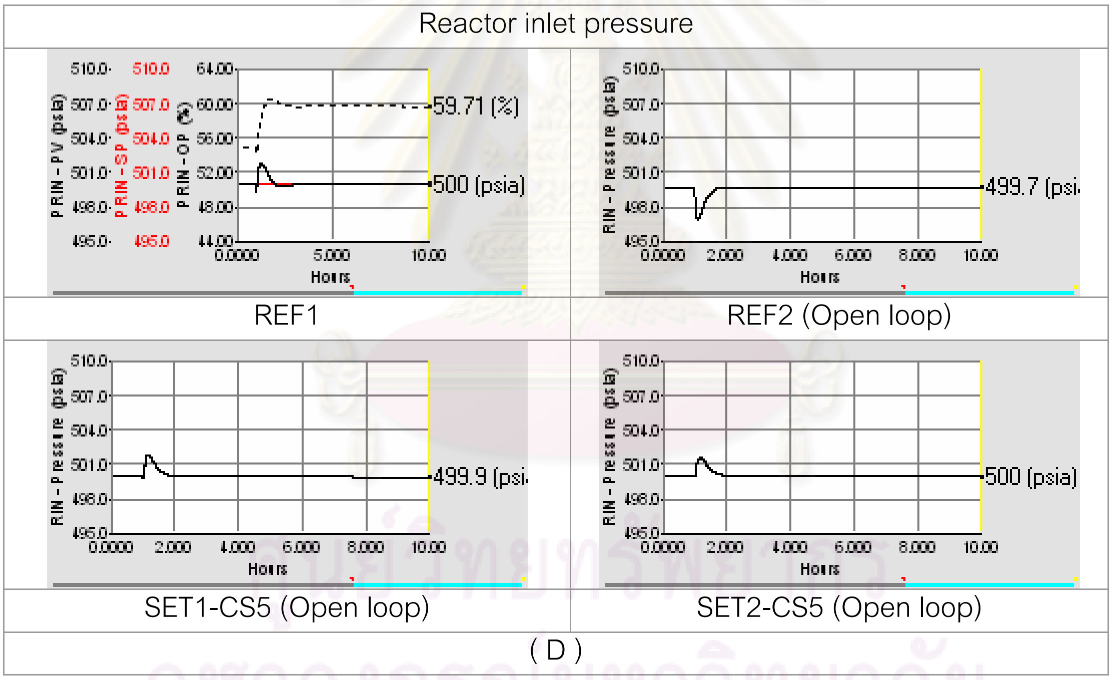
REF1 (Open loop)

REF2

SET1-CS5

SET2-CS5

( C )



Reactor inlet pressure

REF1

REF2 (Open loop)

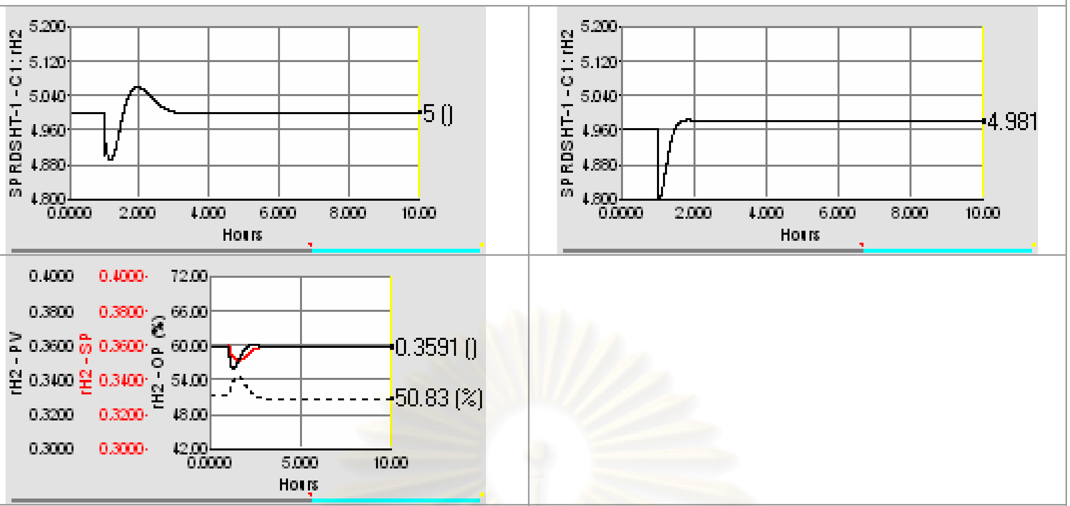
SET1-CS5 (Open loop)

SET2-CS5 (Open loop)

( D )

**Figure 5.14** Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

Hydrogen to aromatic ratio at reactor inlet (rH2)



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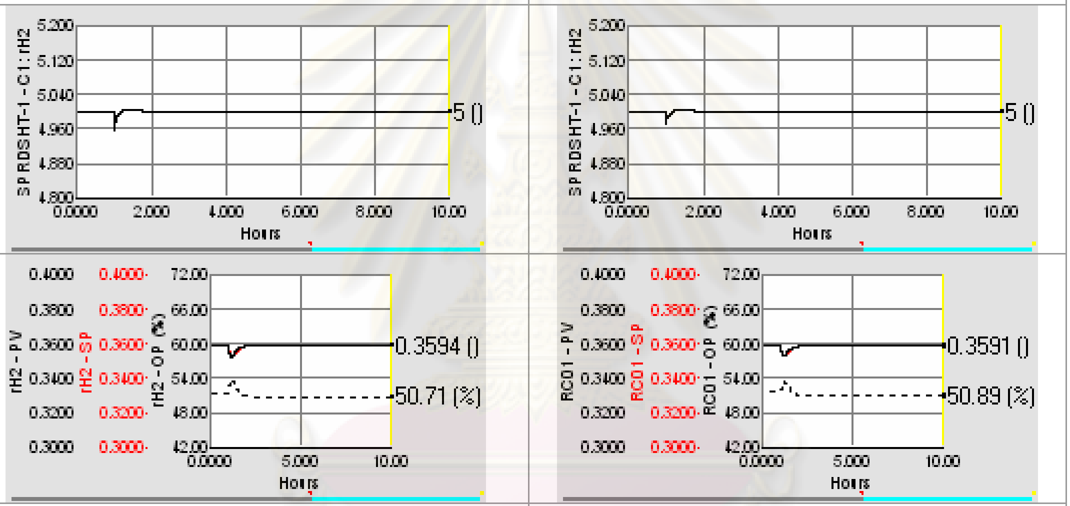


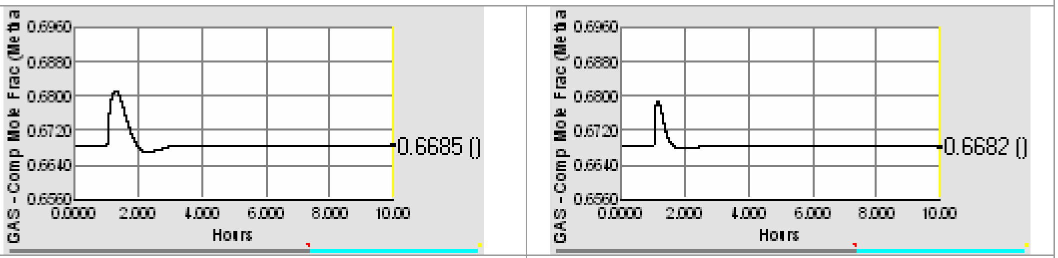
SET1-CS5

SET2-CS5

( E )

Figure 5.14 Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

Methane mole fraction on vapor separator stream



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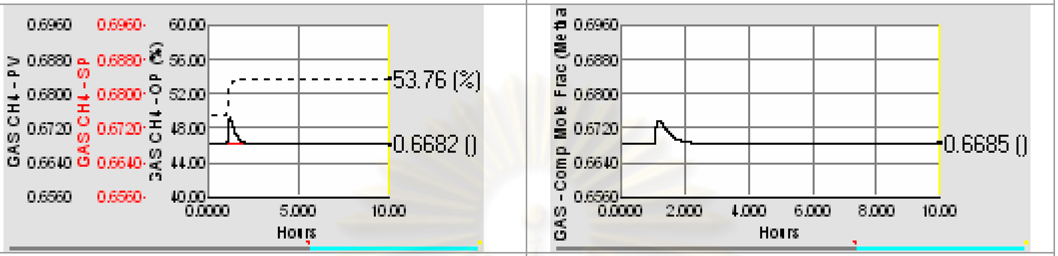
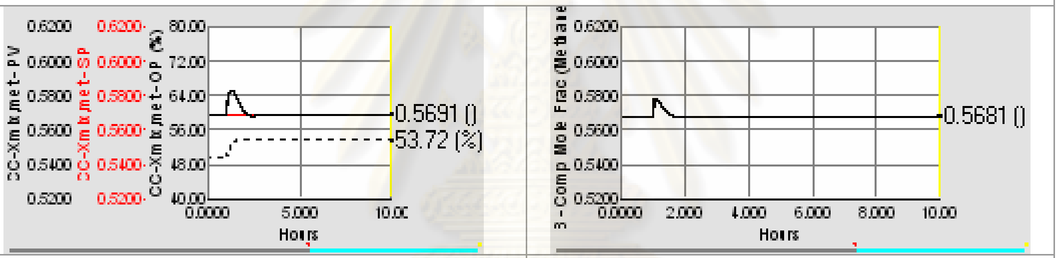


SET1-CS5 SET2-CS5 (Open loop)

( F )

Methane mole fraction on mixture outlet stream



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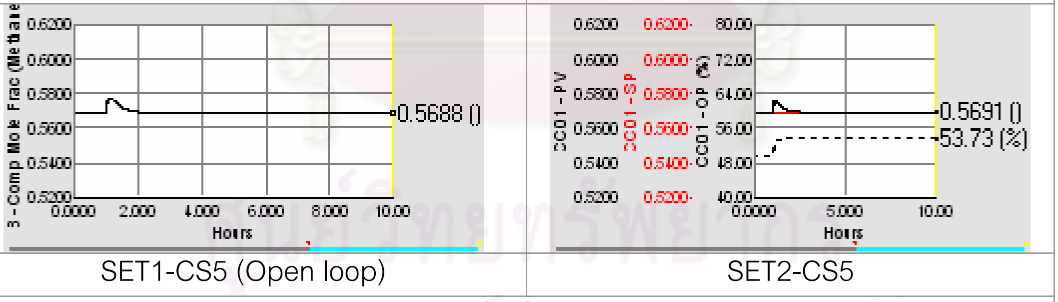
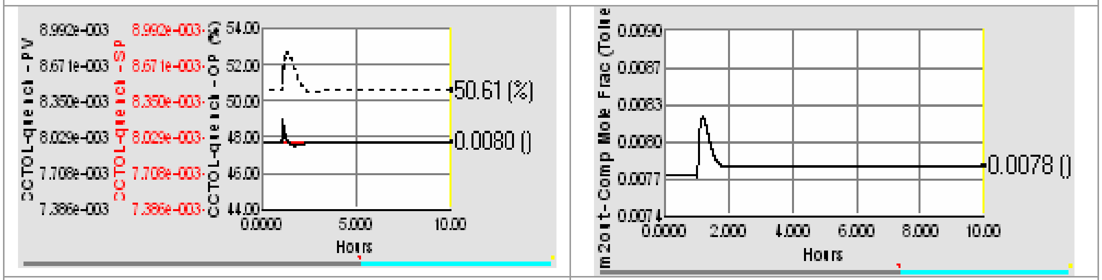


SET1-CS5 (Open loop) SET2-CS5

( G )

Figure 5.14 Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

Toluene mole fraction in quencher outlet stream



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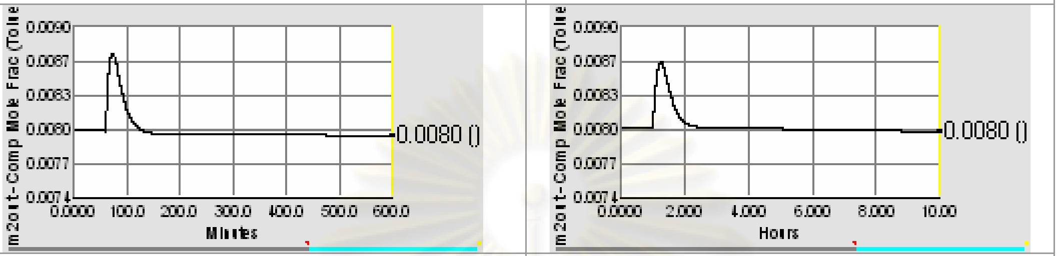
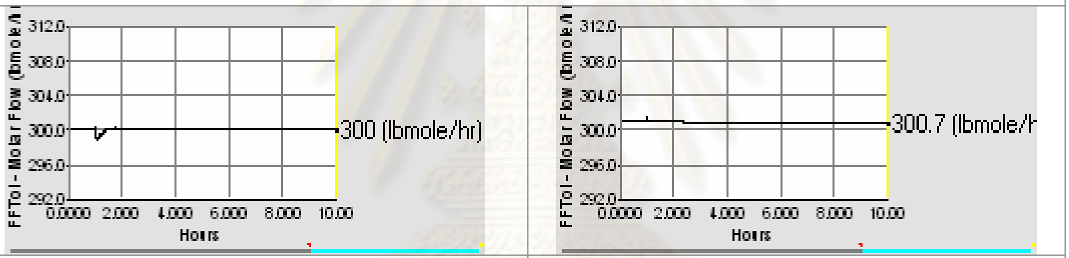


SET1-CS5 (Open loop) SET2-CS5 (Open loop)

( H )

Manipulated variable 1 : Fresh toluene feed rate



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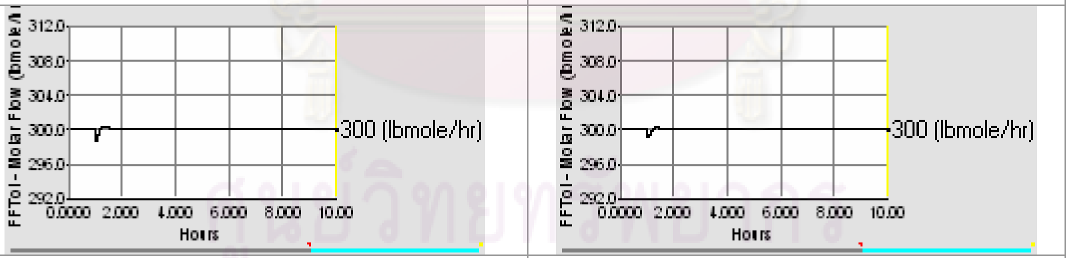

SET1-CS5 SET2-CS5

( I )

**Figure 5.14** Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

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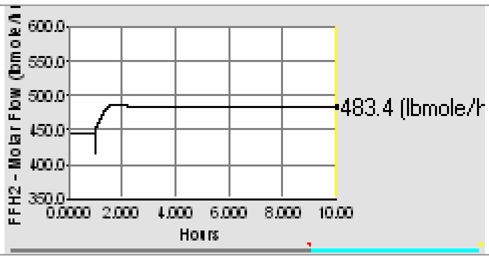
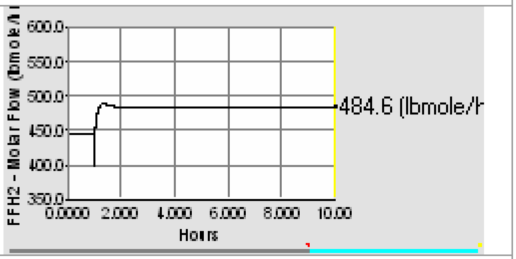
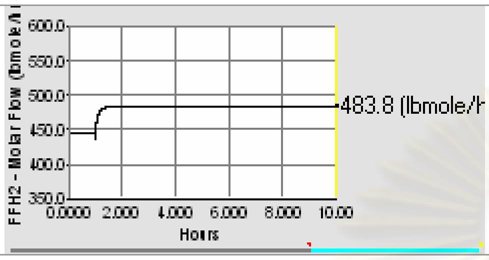
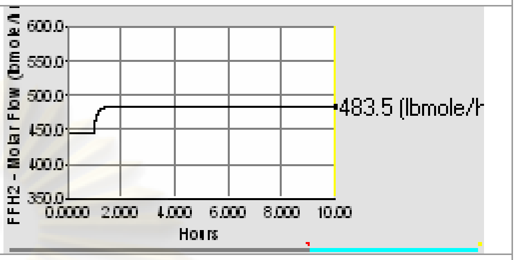
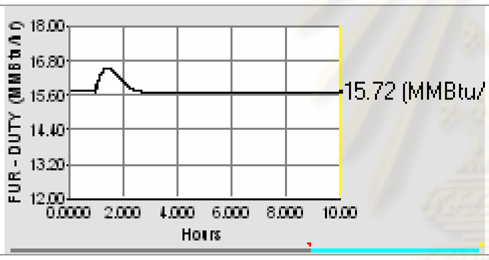
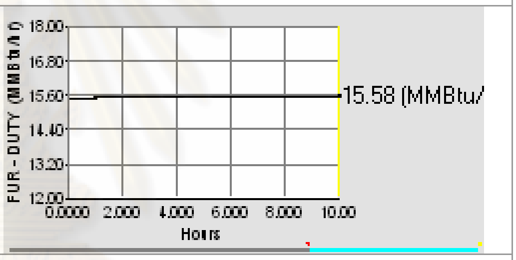
|  |  |
| REF1 | REF2 |
|  |  |
| SET1-CS5 | SET2-CS5 |
| ( J ) | |

| Manipulated variable 3 : Furnace heat duty | |
|---|---|
|  |  |
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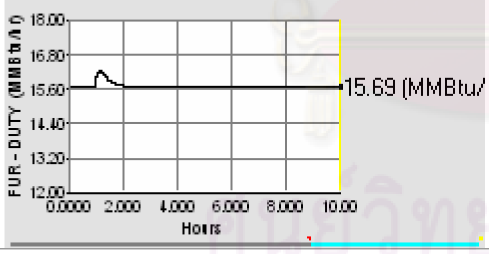
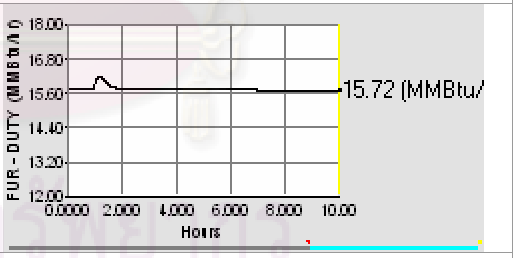
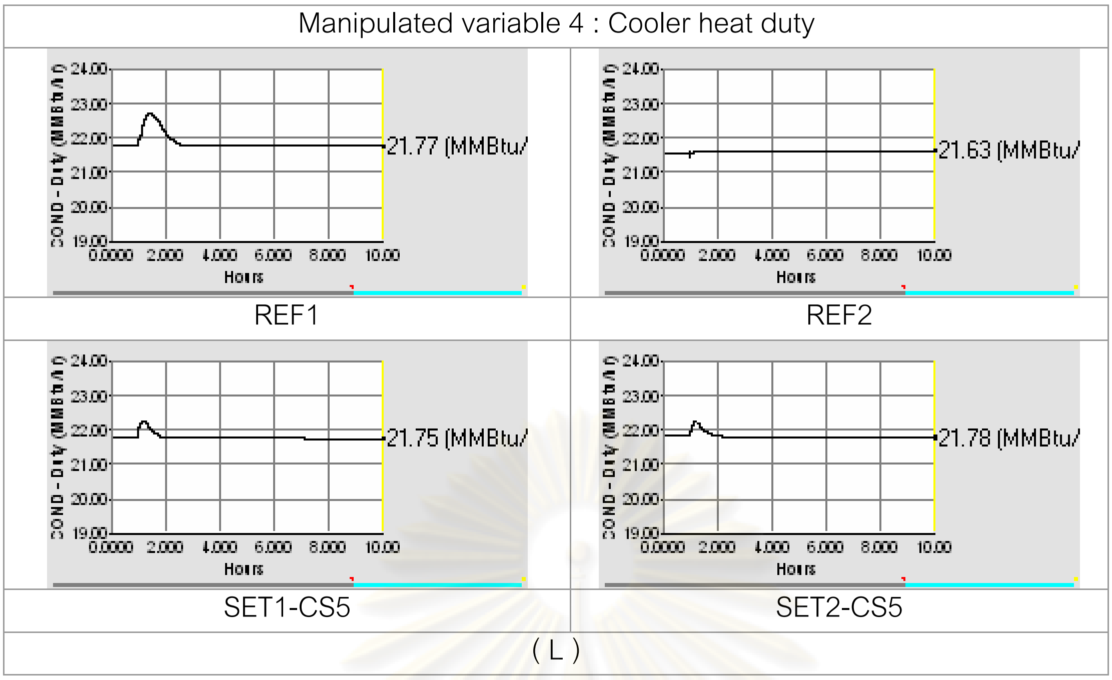
|  |  |
| SET1-CS5 | SET2-CS5 |
| ( K ) | |

Figure 5.14 Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

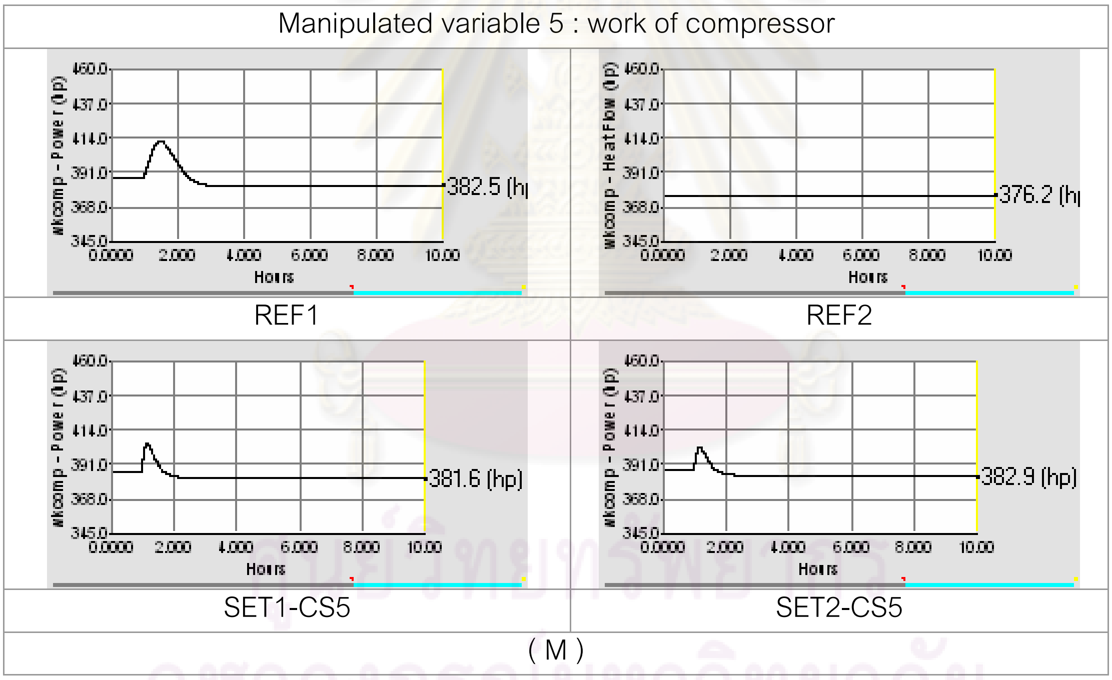


Manipulated variable 4 : Cooler heat duty

REF1 REF2

SET1-CS5 SET2-CS5

( L )



Manipulated variable 5 : work of compressor

REF1 REF2

SET1-CS5 SET2-CS5

( M )

Figure 5.14 Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

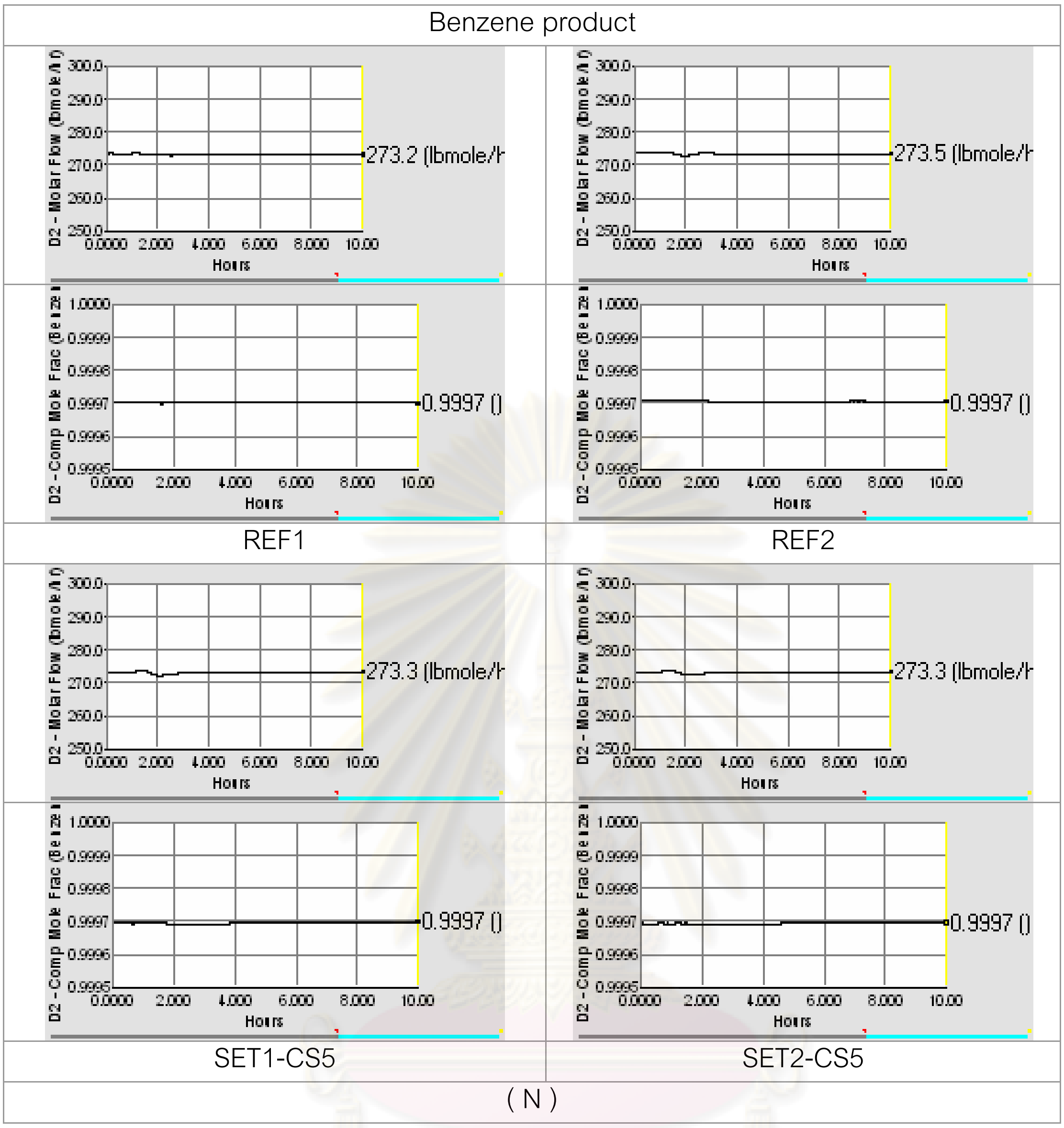


Figure 5.14 Dynamic responses of increase methane mole fraction in fresh feed gas for; (A) Quencher outlet temperature, (B) Reactor inlet temperature, (C) Separator pressure, (D) Reactor inlet pressure, (E) Hydrogen to aromatic ratio at reactor inlet, (F) Methane mole fraction on vapor separator stream, (G) Methane composition in separator vapor stream, (H) Toluene mole fraction in quencher outlet stream, (I) Fresh feed toluene, (J) Fresh feed hydrogen, (K) Furnace heat duty, (L) Cooler heat duty, (M) Work of compressor and (N) Benzene product

# CHAPTER VI

# CONCLUSION AND SUGGESTION FOR FURTHER WORK

## 6.1 Conclusion

In this research has discussed control structure design for the HDA process, using the design procedure of Wongsri (2008). The process variables should be control are selected by the “fixture point theorem”. The procedure is base on the selection of controlled variable that the most disturbances propagate to plantwide, previously using heuristic approach. The maximum (scale) gain is used to paring controlled variables with manipulated variables. Table 6.1 shows the set of controlled variables of this work compare with various authors.

**Table 6.1** Controlled variables selected by various authors (Reaction Section)

| Controlled variable | authors | | | |
|---|---|---|---|---|
| | 1 | 2 | 3 | 4* |
| Fresh toluene feed rate (FFTOL) | | X | X | X |
| Fresh gas hydrogen feed rate (FFH2) | | | | X |
| Recycle gas methane mole fraction | X | | | |
| Reactor inlet pressure (Prin) | | X | X | |
| Compressor power | X | | | |
| Total toluene flow rate to the reaction section | X | | | |
| Mixer outlet methane mole fraction (Xmet,mix) | | X | | |
| Reactor inlet temperature (Trin) | X | X | X | X |
| Reactor outlet temperature (Trout) | | | X | |
| Separator temperature | X | X | X | X |
| Separator pressure | X | | | X |
| Separator overhead vapor methane mole fraction | | | X | X |
| Hydrogen to aromatic ratio at reactor inlet (rH2) | | X | X | X |
| Quencher outlet temperature | X | X | X | X |
| Quencher outlet toluene mole fraction | | X | | |

**Note:** 1=Luyben (1998), 2=Araujo et al.(2006) 3=Chotirat Kiatpiriya (reaction section only, 2007), 4*= This work

From this work we can conclusion

1. Easy for pre-screening output from input (MV and D are considered).
2. The appropriate set of controlled variables to achieve form fixture point theorem.
3. The best control configurations depend on the direction of controlled variable with manipulated variable.

## 6.2 Recommendations

The Fixture point theorem is the easy and effective tool to select controlled variables. The fixture point is effective with the plantwide level. Therefore we will improve steps of plantwide control structure design procedure correspond to the fixture point theorem.

# REFERENCES

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# APPENDICES

# APPENDIX A

# TUNING OF CONTROL STRUCTURES

## A.1 Tuning Controllers

Notice throughout this work uses several types of controllers such as P, PI, and PID controllers. They depend on the control loop. In theory, control performance can be improved by the use of derivative action but in practice the use of derivative has some significant drawbacks:

1. Three tuning constants must be specified.
2. Signal noise is amplified.
3. Several types of PID control algorithms are used, so important to careful that the right algorithm is used with its matching tuning method.
4. The simulation is an approximation of the real plant. If high performance controllers are required to get good dynamics from the simulation, the real plant may not work well.

## A.2 Tuning Flow, Level and Pressure Loops

The dynamics of flow measurement are fast. The time constants for moving control valves are small. Therefore, the controller can be turned with a small integral or reset time constant. A value of $\tau_I$ = 0.3 minutes work in most controllers. The value of controller gain should be kept modest because flow measurement signal are sometime noisy due to the turbulent flow through the orifice plate. A value of controller gain of $K_C$ = 0.5 is often used. Derivative action should not be used.

Most level controllers should use proportional-only action with a gain of 1 to 2. This provides the maximum amount of flow smoothing. Proportional control means there will be steady state offset (the level will not be returned to its setpoint value). However, maintaining a liquid level at a certain value is often not necessary when the liquid capacity is simply being used as surge volume. So the recommended tuning of a level controller is $K_C$ = 2.

Most pressure controllers can be fairly easily tuned. The process time constant is estimated by dividing the gas volume of the system by the volumetric flowrate of gas flowing through the system. Setting the integral time equal to about 2 to 4 times the process time constant and using a reasonable controller gain usually gives satisfactory pressure control. Typical pressure controller tuning constants for columns and tanks are $K_C$ = 2 and $\tau_I$ = 10 minutes.

## A.3 Relay- Feedback Testing

The relay-feedback test is a tool that serves a quick and simple method for identifying the dynamic parameters that are important for to design a feedback controller. The results of the test are the ultimate gain and the ultimate frequency. This information is usually sufficient to permit us to calculate some reasonable controller tuning constants.

The method consists of merely inserting an on-off relay in the feedback loop. The only parameter that must be specified is the height of the relay, h. This height is typically 5 to 10 % of the controller output scale. The loop starts to oscillate around the setpoint with the controller output switching every time the process variable (PV) signal crosses the setpoint. Figure A.1 shows the PV and OP signals from a typical relay-feedback test.

The maximum amplitude (a) of the PV signal is used to calculate the ultimate gain, $K_U$ from the equation

$$K_U = \frac{4h}{a\pi} \qquad \text{(A.1)}$$

The period of the output PV curve is the ultimate period, $P_U$ from these two parameters controller tuning constants can be calculated for PI and PID controllers, using a variety of tuning methods proposed in the literature that require only the ultimate gain and the ultimate frequency, e.g. Ziegler-Nichols, Tyreus-Luyben.

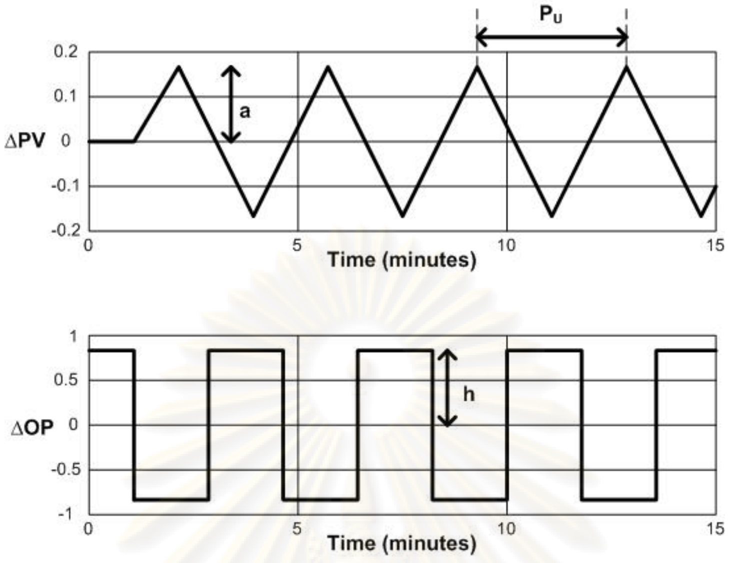


**Figure A.1** Input and Output from Relay-Feedback Test

The test has many positive features that have led to its widespread use in real plants as well in simulation studies:

1. Only one parameter has to be specified (relay height).
2. The time it takes to run the test is short, particularly compared to the extended periods required for methods like PRBS.
3. The test is closedloop, so the process is not driven away from the setpoint.
4. The information obtained is very accurate in the frequency range that is important for the design of a feedback controller.
5. The impact of load changes that occur during the test can be detected by a change to asymmetric pulses in the manipulated variable.

These entire features make relay-feedback testing a useful identification tool. Knowing the ultimate gain, $K_U$ and the ultimate period, $P_U$ permits us to calculate controller settings. There are several methods that require only these two parameters. The Ziegler-Nichols tuning equations for a PI controller are:

$$\begin{aligned} K_C &= K_U / 2.2 \\ \tau_I &= P_U / 1.2 \end{aligned} \qquad \text{(A.2)}$$

These tuning constants are frequently too aggressive for many chemical engineering applications. The Tyreus-Luyben tuning method provides more conservative settings with increased robustness. The TL equations for a PI controller are:

$$\begin{aligned} K_C &= K_U / 3.2 \\ \tau_I &= 2.2 P_U \end{aligned} \qquad \text{(A.3)}$$

## A.4 Inclusion of Lags

Any real physical system has many lags. Measurement and actuator lags always exist. In simulations, however, these lags are not part of the unit models. Much more aggressive tuning is often possible on the simulation than is possible in the real plant. Thus the predictions of dynamic performance can be overly optimistic. This is poor engineering. A conservative design is needed.

Realistic dynamic simulations require that we explicitly include lags and/or dead times in all the important loops. Usually this means controllers that affect Product quality or process constraint.

Table A.1 summarizes some recommended lags to include in several different types of control loops.

**Table A.1** Typical measurement lags

| | | Number | Time constant (minutes) | Type |
|---|---|---|---|---|
| Temperature | Liquid | 2 | 0.5 | First-order lags |
| | Gas | 3 | 1 | First-order lags |
| Composition | Chromatograph | 1 | 3 to 10 | Deadtime |

# APPENDIX B

## PARAMETER TUNING

**Table B.1** Tuning parameters for the reference control structure 1 (REF1)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| TC01 | Quencher outlet temperature | V6 | 0.1 | 0.1 | - | Direct | 1100-1200 F |
| TC02 | Reactor inlet temperature | Qfur | 2 | 10 | - | Reverse | 1100-1300 F |
| TC03 | Separator inlet temperature | Qcooler | 1.36 | 0.8 | - | Direct | 70-120 F |
| RC01 | Hydrogen to aromatic ratio at reactor inlet | Wkcomp | 0.27 | 2.86 | - | Reverse | 0.1091-0.6091 |
| PC-RIN | Reactor inlet pressure | V5 | 2 | 10 | - | Direct | 400-600 psia |
| CC01 | Mixer outlet methane mole fraction | SP FC-01 | 0.54 | 12.5 | - | Direct | 0.3190-0.8190 |
| CC02 | Quencher outlet toluene mole fraction | SP TC-02 | 0.69 | 2.93 | - | Direct | 0.000-0.016 |
| LC-SEP | Separator liquid level | V4 | 2 | - | - | Direct | 0-100 % |
| LC1 | Reflux drum level of stabilizer column | qc1 | 2 | - | - | Reverse | 0-100 % |
| LC2 | Reflux drum level of benzene column | V13 | 2 | - | - | Direct | 0-100 % |
| LC3 | Reflux drum level of toluene column | V10 | 2 | - | - | Direct | 0-100 % |
| LRC1 | Reboiler sump level of stabilizer column | V12 | 2 | - | - | Direct | 0-100 % |
| LRC2 | Reboiler sump level of benzene column | V14 | 2 | - | - | Direct | 0-100 % |
| LRC3 | Reboiler sump level of toluene column | V15 | 2 | - | - | Direct | 0-100 % |

**Table B.1** (Continuous) Tuning parameters for the reference control structure 1 (REF1)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| PC1 | Condenser pressure of stabilizer column | V11 | 2 | 10 | - | Direct | 100-200 psia |
| PC2 | Condenser pressure of benzene column | qc2 | 2 | 10 | - | Direct | 20-40 psia |
| PC3 | Condenser pressure of toluene column | qc3 | 2 | 10 | - | Direct | 20-40 psia |
| C1 TS-3 | Temperature at tray 3 in stabilizer column | qr1 | 2 | 10 | - | Reverse | 273.18-373.18 F |
| C2 TS-20 | Temperature at tray 20 in benzene column | qr2 | 2 | 10 | - | Reverse | 194.84-294.84 F |
| C3 TS-5 | Temperature at tray 5 in toluene column | Reflux rate | 0.1 | 0.1 | - | Direct | 258.54-358.54 F |
| CC11 | Benzene mole fraction in distillate of stabilizer column | Reflux rate | 1 | 50 | - | Direct | 0.000-0.002 |
| CC12 | Methane mole fraction in bottoms of stabilizer column | SP C1 TS-3 | 1.5 | 50 | - | Direct | 0.0-2.0E-06 |
| CC21 | Toluene mole fraction in distillate of benzene column | Reflux rate | 1 | 50 | - | Direct | 0.0-6.0E-04 |
| CC22 | Benzene mole fraction in bottoms of benzene column | SP C2 TS-20 | 1.5 | 50 | - | Direct | 0.0-2.6E-03 |
| CC31 | Biphenyl mole fraction in distillate of toluene column | SP C3-TS5 | 7.5E-02 | 100 | - | Reverse | 0.0-1.0E-03 |
| CC32 | Toluene mole fraction in bottoms of toluene column | qr3 | 1 | 50 | - | Direct | 0.0-8.0E-04 |
| FC01 | Fresh hydrogen feed flowrate | V1 | 0.5 | 0.3 | - | Reverse | 0-900 lbmole/hr |
| FC02 | Fresh toluene feed flowrate | V2 | 0.5 | 0.3 | - | Reverse | 0-600 lbmole/hr |

**Table B.2** Tuning parameters for the reference control structure 2 (REF2)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| TC01 | Quencher outlet temperature | V6 | 0.1 | 0.1 | - | Direct | 1100-1200 F |
| TC02 | Reactor inlet temperature | Qfur | 2 | 10 | - | Reverse | 1100-1300 F |
| TC03 | Separator inlet temperature | Qcooler | 2 | 10 | - | Direct | 70-120 F |
| PC-SEP | Separator pressure | V1 | 1 | 10 | - | Reverse | 427-527 psia |
| CC-RCH4 | Compressor inlet methane mole fraction | V5 | 0.5 | 15 | - | Direct | 0.4682-0.8682 |
| LC-SEP | Separator liquid level | V4 | 3 | - | - | Direct | 0-100 % |
| LC1 | Reflux drum level of stabilizer column | qc1 | 2 | - | - | Reverse | 0-100 % |
| LC2 | Reflux drum level of benzene column | V13 | 2 | - | - | Direct | 0-100 % |
| LC3 | Reflux drum level of toluene column | V10 | 3 | - | - | Direct | 0-100 % |
| LRC1 | Reboiler sump level of stabilizer column | V12 | 2 | - | - | Direct | 0-100 % |
| LRC2 | Reboiler sump level of benzene column | V14 | 2 | - | - | Direct | 0-100 % |
| LRC3 | Reboiler sump level of toluene column | qr3 | 3 | - | - | Direct | 0-100 % |
| PC1 | Condenser pressure of stabilizer column | V11 | 2 | 10 | - | Direct | 100-200 psia |
| PC2 | Condenser pressure of benzene column | qc2 | 2 | 10 | - | Direct | 20-40 psia |
| PC3 | Condenser pressure of toluene column | qc3 | 5 | 10 | - | Direct | 20-40 psia |
| C1 TS-6 | Temperature at tray 6 in stabilizer column | qr1 | 2 | 10 | - | Reverse | 241.38-341.38 F |
| C2 TS-12 | Temperature at tray 12 in benzene column | qr2 | 2 | 10 | - | Reverse | 183.59-283.59 F |
| C3 TS-Avg | Average trays temperature ( tray 1-4 ) in toluene column | V15 | 1 | 30 | - | Direct | 357.64-557.64 F |
| FC-TOT | Total toluene feed flowrate | V2 | 0.5 | 0.3 | - | Reverse | 0-800 lbmole/hr |

Table B.3 Tuning parameters for the control structure 1 (CS1)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| TC01 | Quencher outlet temperature | V6 | 0.1 | 0.1 | - | Direct | 1100-1200 F |
| TC02 | Reactor inlet temperature | Qfur | 2 | 10 | - | Reverse | 1100-1300 F |
| TC03 | Separator inlet temperature | Qcooler | 2 | 10 | - | Direct | 70-120 F |
| RC01 | Hydrogen to aromatic ratio at reactor inlet | SP FC-02 | 1 | 0.8 | - | Direct | 0.1091-0.6091 |
| PC-SEP | Separator pressure | SP FC-01 | 2 | 10 | - | Reverse | 427-527 psia |
| CC-GCH4 | Separator vapor methane mole fraction | V5 | 1.5 | 15 | - | Direct | 0.4682-0.8682 |
| LC-SEP | Separator liquid level | V4 | 2 | - | - | Direct | 0-100 % |
| LC1 | Reflux drum level of stabilizer column | qc1 | 2 | - | - | Reverse | 0-100 % |
| LC2 | Reflux drum level of benzene column | V13 | 2 | - | - | Direct | 0-100 % |
| LC3 | Reflux drum level of toluene column | V10 | 2 | - | - | Direct | 0-100 % |
| LRC1 | Reboiler sump level of stabilizer column | V12 | 2 | - | - | Direct | 0-100 % |
| LRC2 | Reboiler sump level of benzene column | V14 | 2 | - | - | Direct | 0-100 % |
| LRC3 | Reboiler sump level of toluene column | V15 | 2 | - | - | Direct | 0-100 % |
| PC1 | Condenser pressure of stabilizer column | V11 | 2 | 10 | - | Direct | 100-200 psia |
| PC2 | Condenser pressure of benzene column | qc2 | 2 | 10 | - | Direct | 20-40 psia |
| PC3 | Condenser pressure of toluene column | qc3 | 2 | 10 | - | Direct | 20-40 psia |
| C1 TS-6 | Temperature at tray 6 in stabilizer column | qr1 | 2 | 10 | - | Reverse | 241.38-341.38 F |
| C2 TS-10 | Temperature at tray 10 in benzene column | qr2 | 2 | 10 | - | Reverse | 194.84-294.84 F |
| C3 TS-4 | Temperature at tray 4 in toluene column | qr3 | 2 | 10 | - | Reverse | 277.73-377.73 F |
| FC-01 | Fresh hydrogen feed flowrate | V1 | 0.179 | 8.36E-03 | - | Reverse | 0-900 lbmole/hr |
| FC-02 | Fresh toluene feed flowrate | V2 | 0.174 | 8.38E-03 | - | Reverse | 0-600 lbmole/hr |

**Table B.4** Tuning parameters for the control structure 2 (CS2)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| TC01 | Quencher outlet temperature | V6 | 0.1 | 0.1 | - | Direct | 1100-1200 F |
| TC02 | Reactor inlet temperature | Qfur | 2 | 10 | - | Reverse | 1100-1300 F |
| TC03 | Separator inlet temperature | Qcooler | 2 | 10 | - | Direct | 70-120 F |
| RC01 | Hydrogen to aromatic ratio at reactor inlet | SP FC-02 | 1 | 0.8 | - | Direct | 0.1091-0.6091 |
| PC-SEP | Separator pressure | V5 | 2 | 10 | - | Direct | 427-527 psia |
| CC-GCH4 | Separator vapor methane mole fraction | SP FC-01 | 1.5 | 15 | - | Direct | 0.4682-0.8682 |
| LC-SEP | Separator liquid level | V4 | 2 | - | - | Direct | 0-100 % |
| LC1 | Reflux drum level of stabilizer column | qc1 | 2 | - | - | Reverse | 0-100 % |
| LC2 | Reflux drum level of benzene column | V13 | 2 | - | - | Direct | 0-100 % |
| LC3 | Reflux drum level of toluene column | V10 | 2 | - | - | Direct | 0-100 % |
| LRC1 | Reboiler sump level of stabilizer column | V12 | 2 | - | - | Direct | 0-100 % |
| LRC2 | Reboiler sump level of benzene column | V14 | 2 | - | - | Direct | 0-100 % |
| LRC3 | Reboiler sump level of toluene column | V15 | 2 | - | - | Direct | 0-100 % |
| PC1 | Condenser pressure of stabilizer column | V11 | 2 | 10 | - | Direct | 100-200 psia |
| PC2 | Condenser pressure of benzene column | qc2 | 2 | 10 | - | Direct | 20-40 psia |
| PC3 | Condenser pressure of toluene column | qc3 | 2 | 10 | - | Direct | 20-40 psia |
| C1 TS-6 | Temperature at tray 6 in stabilizer column | qr1 | 2 | 10 | - | Reverse | 241.38-341.38 F |
| C2 TS-10 | Temperature at tray 10 in benzene column | qr2 | 2 | 10 | - | Reverse | 194.84-294.84 F |
| C3 TS-4 | Temperature at tray 4 in toluene column | qr3 | 2 | 10 | - | Reverse | 277.73-377.73 F |
| FC01 | Fresh hydrogen feed flowrate | V1 | 0.179 | 8.36E-03 | - | Reverse | 0-900 lbmole/hr |
| FC02 | Fresh toluene feed flowrate | V2 | 0.174 | 8.38E-03 | - | Reverse | 0-600 lbmole/hr |

**Table B.5** Tuning parameters for the control structure 3 (CS3)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| TC01 | Quencher outlet temperature | V6 | 0.1 | 0.1 | - | Direct | 1100-1200 F |
| TC02 | Reactor inlet temperature | Qfur | 2 | 10 | - | Reverse | 1100-1300 F |
| TC03 | Separator inlet temperature | Qcooler | 2 | 10 | - | Direct | 70-120 F |
| RC01 | Hydrogen to aromatic ratio at reactor inlet | SP FC-01 | 1 | 0.8 | - | Reverse | 0.1091-0.6091 |
| PC-SEP | Separator pressure | Wkcomp | 2 | 10 | - | Direct | 427-527 psia |
| CC-GCH4 | Separator vapor methane mole fraction | V5 | 1.5 | 15 | - | Direct | 0.4682-0.8682 |
| LC-SEP | Separator liquid level | V4 | 2 | - | - | Direct | 0-100 % |
| LC1 | Reflux drum level of stabilizer column | qc1 | 2 | - | - | Reverse | 0-100 % |
| LC2 | Reflux drum level of benzene column | V13 | 2 | - | - | Direct | 0-100 % |
| LC3 | Reflux drum level of toluene column | V10 | 5 | - | - | Direct | 0-100 % |
| LRC1 | Reboiler sump level of stabilizer column | V12 | 2 | - | - | Direct | 0-100 % |
| LRC2 | Reboiler sump level of benzene column | V14 | 2 | - | - | Direct | 0-100 % |
| LRC3 | Reboiler sump level of toluene column | V15 | 2 | - | - | Direct | 0-100 % |
| PC1 | Condenser pressure of stabilizer column | V11 | 2 | 10 | - | Direct | 100-200 psia |
| PC2 | Condenser pressure of benzene column | qc2 | 2 | 10 | - | Direct | 20-40 psia |
| PC3 | Condenser pressure of toluene column | qc3 | 2 | 10 | - | Direct | 20-40 psia |
| C1 TS-6 | Temperature at tray 6 in stabilizer column | qr1 | 2 | 10 | - | Reverse | 241.38-341.38 F |
| C2 TS-10 | Temperature at tray 10 in benzene column | qr2 | 2 | 10 | - | Reverse | 194.84-294.84 F |
| C3 TS-4 | Temperature at tray 4 in toluene column | qr3 | 2 | 10 | - | Reverse | 277.73-377.73 F |
| FC01 | Fresh hydrogen feed flowrate | V1 | 0.182 | 8.35E-03 | - | Reverse | 0-900 lbmole/hr |
| FC02 | Fresh toluene feed flowrate | V2 | 0.5 | 0.3 | - | Reverse | 0-600 lbmole/hr |

**Table B.6** Tuning parameters for the control structure 4 (CS4)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| TC01 | Quencher outlet temperature | V6 | 0.1 | 0.1 | - | Direct | 1100-1200 F |
| TC02 | Reactor inlet temperature | Qfur | 2 | 10 | - | Reverse | 1100-1300 F |
| TC03 | Separator inlet temperature | Qcooler | 2 | 10 | - | Direct | 70-120 F |
| RC01 | Hydrogen to aromatic ratio at reactor inlet | Wkcomp | 1 | 0.8 | - | Reverse | 0.1091-0.6091 |
| PC-SEP | Separator pressure | SP FC-01 | 2 | 10 | - | Reverse | 427-527 psia |
| CC-GCH4 | Separator vapor methane mole fraction | V5 | 1.5 | 15 | - | Direct | 0.4682-0.8682 |
| LC-SEP | Separator liquid level | V4 | 2 | - | - | Direct | 0-100 % |
| LC1 | Reflux drum level of stabilizer column | qc1 | 2 | - | - | Reverse | 0-100 % |
| LC2 | Reflux drum level of benzene column | V13 | 2 | - | - | Direct | 0-100 % |
| LC3 | Reflux drum level of toluene column | V10 | 5 | - | - | Direct | 0-100 % |
| LRC1 | Reboiler sump level of stabilizer column | V12 | 2 | - | - | Direct | 0-100 % |
| LRC2 | Reboiler sump level of benzene column | V14 | 2 | - | - | Direct | 0-100 % |
| LRC3 | Reboiler sump level of toluene column | V15 | 2 | - | - | Direct | 0-100 % |
| PC1 | Condenser pressure of stabilizer column | V11 | 2 | 10 | - | Direct | 100-200 psia |
| PC2 | Condenser pressure of benzene column | qc2 | 2 | 10 | - | Direct | 20-40 psia |
| PC3 | Condenser pressure of toluene column | qc3 | 2 | 10 | - | Direct | 20-40 psia |
| C1 TS-6 | Temperature at tray 6 in stabilizer column | qr1 | 2 | 10 | - | Reverse | 241.38-341.38 F |
| C2 TS-10 | Temperature at tray 10 in benzene column | qr2 | 2 | 10 | - | Reverse | 194.84-294.84 F |
| C3 TS-4 | Temperature at tray 4 in toluene column | qr3 | 2 | 10 | - | Reverse | 277.73-377.73 F |
| FC01 | Fresh hydrogen feed flowrate | V1 | 0.184 | 8.34E-03 | - | Reverse | 0-900 lbmole/hr |
| FC02 | Fresh toluene feed flowrate | V2 | 0.5 | 0.3 | - | Reverse | 0-600 lbmole/hr |

Table B.7 Tuning parameters for the control structure 5 (CS5)

| Controller | Controlled variables | Manipulated variable | Tuning parameter | | | Action controller | PV Range |
|---|---|---|---|---|---|---|---|
| | | | $K_C$ | $\tau_I$ | $\tau_D$ | | |
| TC01 | Quencher outlet temperature | V6 | 0.1 | 0.1 | - | Direct | 1100-1200 F |
| TC02 | Reactor inlet temperature | Qfur | 2 | 10 | - | Reverse | 1100-1300 F |
| TC03 | Separator inlet temperature | Qcooler | 2 | 10 | - | Direct | 70-120 F |
| RC01 | Hydrogen to aromatic ratio at reactor inlet | Wkcomp | 1 | 0.8 | - | Reverse | 0.1091-0.6091 |
| PC-SEP | Separator pressure | V5 | 2 | 10 | - | Direct | 427-527 psia |
| CC-GCH4 | Separator vapor methane mole fraction | SP FC-01 | 1.5 | 15 | - | Direct | 0.4682-0.8682 |
| LC-SEP | Separator liquid level | V4 | 2 | - | - | Direct | 0-100 % |
| LC1 | Reflux drum level of stabilizer column | qc1 | 2 | - | - | Reverse | 0-100 % |
| LC2 | Reflux drum level of benzene column | V13 | 2 | - | - | Direct | 0-100 % |
| LC3 | Reflux drum level of toluene column | V10 | 5 | - | - | Direct | 0-100 % |
| LRC1 | Reboiler sump level of stabilizer column | V12 | 2 | - | - | Direct | 0-100 % |
| LRC2 | Reboiler sump level of benzene column | V14 | 2 | - | - | Direct | 0-100 % |
| LRC3 | Reboiler sump level of toluene column | V15 | 2 | - | - | Direct | 0-100 % |
| PC1 | Condenser pressure of stabilizer column | V11 | 2 | 10 | - | Direct | 100-200 psia |
| PC2 | Condenser pressure of benzene column | qc2 | 2 | 10 | - | Direct | 20-40 psia |
| PC3 | Condenser pressure of toluene column | qc3 | 2 | 10 | - | Direct | 20-40 psia |
| C1 TS-6 | Temperature at tray 6 in stabilizer column | qr1 | 2 | 10 | - | Reverse | 241.38-341.38 F |
| C2 TS-10 | Temperature at tray 10 in benzene column | qr2 | 2 | 10 | - | Reverse | 194.84-294.84 F |
| C3 TS-4 | Temperature at tray 4 in toluene column | qr3 | 2 | 10 | - | Reverse | 277.73-377.73 F |
| FC01 | Fresh hydrogen feed flowrate | V1 | 0.186 | 8.33E-03 | - | Reverse | 0-900 lbmole/hr |
| FC02 | Fresh toluene feed flowrate | V2 | 0.5 | 0.3 | - | Reverse | 0-600 lbmole/hr |

# APPENDIX C

## DATA OF FIXTURE POINT ANALYSIS

| **Table C1-1** (Fixture point ) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT1 | FT2 | FT3 | FT4 | FT5 | FT6 | FT7 | FT8 | FT9 | FT10 | FT11 | FT12 | FT13 |
| | IAE value | | | | | | | | | | | | |
| FFTOL Molar Flow | 0.007 | 0.014 | 0.003 | 0.003 | 0.008 | 0.000 | 0.016 | 0.015 | 0.005 | 0.030 | 0.003 | 0.031 | 0.003 |
| FFTOL P | 0.000 | 0.277 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFTOL Temp | 0.000 | 0.000 | 0.064 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS Molar Flow | 0.005 | 0.010 | 0.003 | 0.007 | 0.021 | 0.003 | 0.020 | 0.019 | 0.006 | 0.038 | 0.004 | 0.039 | 0.004 |
| FFGAS P | 0.000 | 0.000 | 0.000 | 0.000 | 0.277 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS Temp | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.064 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC H2 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC CH4 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC Benzene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC Toluene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| Mixer outlet Molar Flow | 0.048 | 0.096 | 0.031 | 0.027 | 0.080 | 0.017 | 0.252 | 0.185 | 0.133 | 0.320 | 0.096 | 0.334 | 0.097 |
| Mixer outlet P | 0.050 | 0.100 | 0.031 | 0.032 | 0.098 | 0.001 | 0.083 | 0.187 | 0.061 | 0.366 | 0.042 | 0.383 | 0.039 |
| Mixer outlet Temp | 0.038 | 0.076 | 0.050 | 0.006 | 0.015 | 0.016 | 0.044 | 0.292 | 0.068 | 0.368 | 0.098 | 0.389 | 0.096 |
| Mixer outlet_CC H2 | 0.051 | 0.100 | 0.017 | 0.032 | 0.094 | 0.014 | 0.135 | 0.105 | 0.033 | 0.243 | 0.025 | 0.255 | 0.023 |
| Mixer outlet_CC CH4 | 0.041 | 0.082 | 0.015 | 0.028 | 0.084 | 0.012 | 0.131 | 0.089 | 0.036 | 0.220 | 0.023 | 0.231 | 0.024 |
| Mixer outlet_CC Benzene | 0.003 | 0.005 | 0.003 | 0.000 | 0.001 | 0.001 | 0.005 | 0.018 | 0.005 | 0.029 | 0.007 | 0.031 | 0.007 |
| Mixer outlet_CC Toluene | 0.007 | 0.013 | 0.001 | 0.003 | 0.009 | 0.001 | 0.001 | 0.002 | 0.002 | 0.007 | 0.002 | 0.007 | 0.002 |
| Mixer outlet_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FUR IN Molar Flow | 0.048 | 0.096 | 0.031 | 0.027 | 0.080 | 0.017 | 0.252 | 0.185 | 0.133 | 0.320 | 0.096 | 0.334 | 0.097 |
| FUR IN P | 0.044 | 0.087 | 0.029 | 0.035 | 0.105 | 0.001 | 0.059 | 0.172 | 0.167 | 0.356 | 0.071 | 0.372 | 0.078 |

| Table C1-1 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT1 | FT2 | FT3 | FT4 | FT5 | FT6 | FT7 | FT8 | FT9 | FT10 | FT11 | FT12 | FT13 |
| | IAE value | | | | | | | | | | | | |
| FUR IN Temp | 0.012 | 0.025 | 0.037 | 0.003 | 0.011 | 0.010 | 0.226 | 0.206 | 0.047 | 0.513 | 0.047 | 0.470 | 0.049 |
| FUR IN_CC H2 | 0.050 | 0.100 | 0.017 | 0.032 | 0.094 | 0.014 | 0.135 | 0.105 | 0.032 | 0.243 | 0.025 | 0.255 | 0.023 |
| FUR IN_CCCH4 | 0.041 | 0.082 | 0.015 | 0.028 | 0.084 | 0.012 | 0.131 | 0.089 | 0.035 | 0.220 | 0.023 | 0.231 | 0.024 |
| FUR IN_CC Benzene | 0.003 | 0.005 | 0.003 | 0.000 | 0.001 | 0.001 | 0.005 | 0.018 | 0.005 | 0.029 | 0.007 | 0.031 | 0.007 |
| FUR IN_CC Toluene | 0.007 | 0.013 | 0.001 | 0.003 | 0.009 | 0.001 | 0.001 | 0.002 | 0.002 | 0.007 | 0.002 | 0.007 | 0.002 |
| FUR IN_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| RIN Molar Flow | 0.048 | 0.096 | 0.031 | 0.027 | 0.080 | 0.017 | 0.252 | 0.185 | 0.133 | 0.320 | 0.096 | 0.334 | 0.097 |
| RIN P | 0.035 | 0.070 | 0.035 | 0.040 | 0.122 | 0.001 | 0.055 | 0.203 | 0.114 | 0.380 | 0.143 | 0.402 | 0.140 |
| RIN Temp | 0.003 | 0.010 | 0.038 | 0.008 | 0.025 | 0.009 | 0.253 | 0.209 | 0.068 | 0.496 | 0.054 | 0.520 | 0.050 |
| RIN_CC H2 | 0.050 | 0.100 | 0.017 | 0.032 | 0.094 | 0.014 | 0.135 | 0.104 | 0.032 | 0.242 | 0.025 | 0.254 | 0.023 |
| RIN_CCCH4 | 0.041 | 0.082 | 0.015 | 0.028 | 0.084 | 0.012 | 0.131 | 0.089 | 0.035 | 0.220 | 0.023 | 0.231 | 0.024 |
| RIN_CC Benzene | 0.003 | 0.005 | 0.003 | 0.000 | 0.001 | 0.001 | 0.005 | 0.018 | 0.005 | 0.029 | 0.007 | 0.031 | 0.007 |
| RIN_CC Toluene | 0.007 | 0.013 | 0.001 | 0.003 | 0.009 | 0.001 | 0.001 | 0.002 | 0.002 | 0.007 | 0.002 | 0.007 | 0.002 |
| RIN_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| ROUT Molar Flow | 0.048 | 0.096 | 0.031 | 0.027 | 0.080 | 0.017 | 0.252 | 0.185 | 0.132 | 0.320 | 0.096 | 0.334 | 0.097 |
| ROUT P | 0.037 | 0.074 | 0.036 | 0.040 | 0.120 | 0.001 | 0.057 | 0.208 | 0.112 | 0.387 | 0.141 | 0.410 | 0.133 |
| ROUT Temp | 0.004 | 0.010 | 0.033 | 0.008 | 0.027 | 0.007 | 0.247 | 0.178 | 0.077 | 0.438 | 0.047 | 0.458 | 0.049 |
| ROUT_CC H2 | 0.055 | 0.110 | 0.018 | 0.033 | 0.097 | 0.015 | 0.149 | 0.112 | 0.038 | 0.260 | 0.027 | 0.273 | 0.025 |
| ROUT_CCCH4 | 0.047 | 0.093 | 0.017 | 0.030 | 0.088 | 0.013 | 0.149 | 0.102 | 0.042 | 0.248 | 0.026 | 0.260 | 0.029 |
| ROUT_CC Benzene | 0.007 | 0.013 | 0.003 | 0.002 | 0.005 | 0.001 | 0.014 | 0.020 | 0.003 | 0.037 | 0.004 | 0.039 | 0.004 |
| ROUT_CC Toluene | 0.001 | 0.002 | 0.003 | 0.001 | 0.004 | 0.000 | 0.020 | 0.015 | 0.005 | 0.035 | 0.004 | 0.037 | 0.003 |
| ROUT_CC Diphenyl | 0.001 | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.005 | 0.005 | 0.001 | 0.011 | 0.001 | 0.011 | 0.001 |
| Quencher Molar Flow | 0.051 | 0.101 | 0.031 | 0.028 | 0.083 | 0.017 | 0.246 | 0.184 | 0.128 | 0.317 | 0.092 | 0.330 | 0.093 |
| Quencher P | 0.037 | 0.074 | 0.036 | 0.040 | 0.120 | 0.001 | 0.057 | 0.208 | 0.112 | 0.387 | 0.141 | 0.410 | 0.133 |

| Table C1-1 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT1 | FT2 | FT3 | FT4 | FT5 | FT6 | FT7 | FT8 | FT9 | FT10 | FT11 | FT12 | FT13 |
| | IAE value | | | | | | | | | | | | |
| Quencher Temp | 0.022 | 0.043 | 0.025 | 0.002 | 0.005 | 0.007 | 0.159 | 0.142 | 0.032 | 0.359 | 0.037 | 0.377 | 0.040 |
| Quencher_CC H2 | 0.053 | 0.105 | 0.018 | 0.032 | 0.094 | 0.014 | 0.146 | 0.110 | 0.038 | 0.254 | 0.026 | 0.266 | 0.024 |
| Quencher_CCCH4 | 0.045 | 0.090 | 0.016 | 0.029 | 0.085 | 0.013 | 0.139 | 0.095 | 0.038 | 0.234 | 0.024 | 0.246 | 0.026 |
| Quencher_CC Benzene | 0.005 | 0.011 | 0.005 | 0.001 | 0.002 | 0.002 | 0.028 | 0.028 | 0.006 | 0.054 | 0.006 | 0.057 | 0.006 |
| Quencher_CC Toluene | 0.001 | 0.002 | 0.004 | 0.002 | 0.006 | 0.001 | 0.028 | 0.022 | 0.008 | 0.051 | 0.005 | 0.054 | 0.005 |
| Quencher_CC Diphenyl | 0.001 | 0.002 | 0.001 | 0.000 | 0.000 | 0.000 | 0.008 | 0.008 | 0.002 | 0.017 | 0.002 | 0.017 | 0.002 |
| FEHE HOT-SIDE Molar Flow | 0.051 | 0.101 | 0.031 | 0.028 | 0.083 | 0.017 | 0.246 | 0.184 | 0.128 | 0.316 | 0.092 | 0.330 | 0.093 |
| FEHE HOT-SIDE P | 0.035 | 0.071 | 0.039 | 0.041 | 0.125 | 0.001 | 0.056 | 0.226 | 0.090 | 0.405 | 0.122 | 0.428 | 0.114 |
| FEHE HOT-SIDE Temp | 0.037 | 0.075 | 0.056 | 0.004 | 0.011 | 0.017 | 0.131 | 0.321 | 0.045 | 0.516 | 0.089 | 0.545 | 0.088 |
| FEHE HOT-SIDE_CC H2 | 0.053 | 0.105 | 0.018 | 0.032 | 0.094 | 0.014 | 0.146 | 0.109 | 0.038 | 0.253 | 0.026 | 0.266 | 0.024 |
| FEHE HOT-SIDE_CCCH4 | 0.045 | 0.090 | 0.016 | 0.029 | 0.085 | 0.013 | 0.139 | 0.095 | 0.038 | 0.234 | 0.024 | 0.245 | 0.026 |
| FEHE HOT-SIDE_CC Toluene | 0.001 | 0.002 | 0.004 | 0.002 | 0.006 | 0.001 | 0.028 | 0.022 | 0.008 | 0.051 | 0.005 | 0.054 | 0.005 |
| FEHE HOT-SIDE_CC Diphenyl | 0.001 | 0.002 | 0.001 | 0.000 | 0.000 | 0.000 | 0.008 | 0.008 | 0.002 | 0.017 | 0.002 | 0.017 | 0.002 |
| SEP INLET Molar Flow | 0.051 | 0.101 | 0.031 | 0.028 | 0.083 | 0.017 | 0.246 | 0.184 | 0.128 | 0.316 | 0.092 | 0.330 | 0.093 |
| SEP INLET P | 0.035 | 0.070 | 0.039 | 0.041 | 0.125 | 0.001 | 0.056 | 0.226 | 0.089 | 0.405 | 0.122 | 0.428 | 0.114 |
| SEP INLET Temp | 0.051 | 0.101 | 0.050 | 0.007 | 0.019 | 0.017 | 0.062 | 0.296 | 0.097 | 0.478 | 0.136 | 0.505 | 0.133 |
| SEP INLET_CC H2 | 0.053 | 0.105 | 0.018 | 0.032 | 0.094 | 0.014 | 0.146 | 0.109 | 0.038 | 0.253 | 0.026 | 0.266 | 0.024 |
| SEP INLET_CCCH4 | 0.045 | 0.090 | 0.016 | 0.029 | 0.085 | 0.013 | 0.139 | 0.095 | 0.038 | 0.234 | 0.024 | 0.245 | 0.026 |
| SEP INLET_CC Benzene | 0.005 | 0.011 | 0.005 | 0.001 | 0.002 | 0.002 | 0.027 | 0.028 | 0.006 | 0.054 | 0.006 | 0.057 | 0.006 |
| SEP INLET_CC Toluene | 0.001 | 0.002 | 0.004 | 0.002 | 0.006 | 0.001 | 0.028 | 0.022 | 0.008 | 0.051 | 0.005 | 0.054 | 0.005 |
| SEP INLET_CC Diphenyl | 0.001 | 0.002 | 0.001 | 0.000 | 0.000 | 0.000 | 0.008 | 0.008 | 0.002 | 0.017 | 0.002 | 0.017 | 0.002 |
| SEP GAS Molar Flow | 0.054 | 0.108 | 0.026 | 0.030 | 0.089 | 0.016 | 0.227 | 0.157 | 0.127 | 0.265 | 0.095 | 0.276 | 0.095 |
| SEP GAS P | 0.035 | 0.070 | 0.039 | 0.041 | 0.125 | 0.001 | 0.056 | 0.226 | 0.089 | 0.405 | 0.122 | 0.428 | 0.114 |

| Table C1-1 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT1 | FT2 | FT3 | FT4 | FT5 | FT6 | FT7 | FT8 | FT9 | FT10 | FT11 | FT12 | FT13 |
| | IAE value | | | | | | | | | | | | |
| SEP GAS Temp | 0.051 | 0.101 | 0.050 | 0.007 | 0.019 | 0.017 | 0.062 | 0.296 | 0.097 | 0.477 | 0.136 | 0.505 | 0.133 |
| SEP GAS_CC H2 | 0.057 | 0.113 | 0.020 | 0.034 | 0.101 | 0.016 | 0.161 | 0.123 | 0.040 | 0.285 | 0.029 | 0.299 | 0.027 |
| SEP GAS_CCCH4 | 0.054 | 0.107 | 0.017 | 0.034 | 0.099 | 0.015 | 0.155 | 0.103 | 0.046 | 0.251 | 0.026 | 0.263 | 0.032 |
| SEP GAS_CC Benzene | 0.003 | 0.006 | 0.003 | 0.000 | 0.001 | 0.001 | 0.006 | 0.021 | 0.005 | 0.034 | 0.008 | 0.036 | 0.008 |
| SEP GAS_CC Toluene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 |
| SEP GAS_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| SEP LIQ Molar Flow | 0.004 | 0.007 | 0.005 | 0.002 | 0.006 | 0.001 | 0.019 | 0.027 | 0.005 | 0.051 | 0.006 | 0.053 | 0.005 |
| SEP LIQ P | 0.035 | 0.070 | 0.039 | 0.041 | 0.125 | 0.001 | 0.056 | 0.226 | 0.089 | 0.405 | 0.122 | 0.428 | 0.114 |
| SEP LIQ Temp | 0.051 | 0.101 | 0.050 | 0.007 | 0.019 | 0.017 | 0.062 | 0.296 | 0.097 | 0.477 | 0.136 | 0.505 | 0.133 |
| SEP LIQ_CC H2 | 0.000 | 0.001 | 0.000 | 0.000 | 0.001 | 0.000 | 0.002 | 0.000 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| SEP LIQ_CCCH4 | 0.003 | 0.005 | 0.001 | 0.002 | 0.006 | 0.000 | 0.008 | 0.003 | 0.006 | 0.004 | 0.006 | 0.004 | 0.006 |
| SEP LIQ_CC Benzene | 0.017 | 0.033 | 0.028 | 0.019 | 0.058 | 0.002 | 0.196 | 0.139 | 0.054 | 0.329 | 0.034 | 0.345 | 0.035 |
| SEP LIQ_CC Toluene | 0.007 | 0.014 | 0.041 | 0.017 | 0.054 | 0.007 | 0.279 | 0.217 | 0.076 | 0.500 | 0.053 | 0.524 | 0.049 |
| SEP LIQ_CC Diphenyl | 0.008 | 0.017 | 0.014 | 0.001 | 0.003 | 0.004 | 0.076 | 0.081 | 0.017 | 0.172 | 0.019 | 0.180 | 0.018 |
| COMP INLET Molar Flow | 0.050 | 0.100 | 0.025 | 0.023 | 0.067 | 0.014 | 0.215 | 0.150 | 0.121 | 0.252 | 0.091 | 0.263 | 0.091 |
| COMP INLET P | 0.035 | 0.070 | 0.039 | 0.041 | 0.125 | 0.001 | 0.056 | 0.226 | 0.089 | 0.405 | 0.122 | 0.428 | 0.114 |
| COMP INLET Temp | 0.051 | 0.101 | 0.050 | 0.007 | 0.019 | 0.017 | 0.062 | 0.296 | 0.097 | 0.477 | 0.136 | 0.505 | 0.133 |
| COMP INLET_CC H2 | 0.057 | 0.113 | 0.020 | 0.034 | 0.101 | 0.016 | 0.161 | 0.123 | 0.040 | 0.285 | 0.029 | 0.299 | 0.027 |
| COMP INLET_CCCH4 | 0.054 | 0.107 | 0.017 | 0.034 | 0.099 | 0.015 | 0.155 | 0.103 | 0.046 | 0.251 | 0.026 | 0.263 | 0.032 |
| COMP INLET_CC Benzene | 0.003 | 0.006 | 0.003 | 0.000 | 0.001 | 0.001 | 0.006 | 0.021 | 0.005 | 0.034 | 0.008 | 0.036 | 0.008 |
| COMP INLET_CC Toluene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 |
| COMP INLET_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| GAS RECYCLE Molar Flow | 0.050 | 0.100 | 0.025 | 0.023 | 0.067 | 0.014 | 0.215 | 0.150 | 0.121 | 0.252 | 0.091 | 0.263 | 0.091 |

| Table C1-1 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT1 | FT2 | FT3 | FT4 | FT5 | FT6 | FT7 | FT8 | FT9 | FT10 | FT11 | FT12 | FT13 |
| | IAE value | | | | | | | | | | | | |
| GAS RECYCLE P | 0.050 | 0.100 | 0.031 | 0.032 | 0.098 | 0.001 | 0.201 | 0.187 | 0.061 | 0.366 | 0.042 | 0.383 | 0.039 |
| GAS RECYCLE Temp | 0.052 | 0.103 | 0.050 | 0.008 | 0.021 | 0.017 | 0.071 | 0.296 | 0.088 | 0.477 | 0.127 | 0.504 | 0.124 |
| GAS RECYCLE_CC H2 | 0.057 | 0.113 | 0.020 | 0.034 | 0.101 | 0.016 | 0.161 | 0.123 | 0.040 | 0.285 | 0.029 | 0.299 | 0.027 |
| GAS RECYCLE_CCCH4 | 0.054 | 0.107 | 0.017 | 0.034 | 0.099 | 0.015 | 0.155 | 0.103 | 0.046 | 0.251 | 0.026 | 0.263 | 0.032 |
| GAS RECYCLE_CC Benzene | 0.003 | 0.006 | 0.003 | 0.000 | 0.001 | 0.001 | 0.006 | 0.021 | 0.005 | 0.034 | 0.008 | 0.036 | 0.008 |
| GAS RECYCLE_CC Toluene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 |
| GAS RECYCLE_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| PURGE Molar Flow | 0.004 | 0.008 | 0.001 | 0.007 | 0.022 | 0.002 | 0.012 | 0.007 | 0.006 | 0.013 | 0.004 | 0.014 | 0.005 |
| PURGE P | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| PURGE Temp | 0.050 | 0.100 | 0.050 | 0.007 | 0.019 | 0.017 | 0.061 | 0.294 | 0.097 | 0.473 | 0.136 | 0.500 | 0.133 |
| PURGE_CC H2 | 0.057 | 0.113 | 0.020 | 0.034 | 0.101 | 0.016 | 0.161 | 0.123 | 0.040 | 0.285 | 0.029 | 0.299 | 0.027 |
| PURGE_CCCH4 | 0.054 | 0.107 | 0.017 | 0.034 | 0.099 | 0.015 | 0.155 | 0.103 | 0.046 | 0.251 | 0.026 | 0.263 | 0.032 |
| PURGE_CC Benzene | 0.003 | 0.006 | 0.003 | 0.000 | 0.001 | 0.001 | 0.006 | 0.021 | 0.005 | 0.034 | 0.008 | 0.036 | 0.008 |
| PURGE_CC Toluene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 |
| PURGE_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| TOL RECYCLE Molar Flow | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| TOL RECYCLE P | 0.050 | 0.100 | 0.031 | 0.032 | 0.098 | 0.001 | 0.201 | 0.187 | 0.061 | 0.366 | 0.042 | 0.383 | 0.039 |
| TOL RECYCLE Temp | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| sum IAE | 2.642 | 5.545 | 1.858 | 1.577 | 4.971 | 0.755 | 8.956 | 10.536 | 4.460 | 20.516 | 4.154 | 21.490 | 4.090 |

| Table C1-2 | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT14 | FT15 | FT16 | FT17 | FT18 | FT19 | FT20 | FT21 | FT22 | FT23 | FT24 | FT25 | FT26 |
| | IAE value | | | | | | | | | | | | |
| FFTOL Molar Flow | 0.030 | 0.012 | 0.033 | 0.021 | 0.013 | 0.012 | 0.011 | 0.011 | 0.010 | 0.015 | 0.002 | 0.002 | 0.026 |
| FFTOL P | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFTOL Temp | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS Molar Flow | 0.038 | 0.015 | 0.041 | 0.026 | 0.017 | 0.015 | 0.014 | 0.014 | 0.012 | 0.019 | 0.002 | 0.003 | 0.032 |
| FFGAS P | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS Temp | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC H2 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC CH4 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC Benzene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC Toluene | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FFGAS_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| Mixer outlet Molar Flow | 0.332 | 0.174 | 0.361 | 0.265 | 0.167 | 0.326 | 0.166 | 0.302 | 0.116 | 0.186 | 0.085 | 0.097 | 0.324 |
| Mixer outlet P | 0.370 | 0.147 | 0.402 | 0.258 | 0.164 | 0.144 | 0.139 | 0.139 | 0.117 | 0.183 | 0.024 | 0.029 | 0.315 |
| Mixer outlet Temp | 0.384 | 0.027 | 0.418 | 0.079 | 0.220 | 0.137 | 0.204 | 0.139 | 0.181 | 0.242 | 0.074 | 0.085 | 0.129 |
| Mixer outlet_CC H2 | 0.245 | 0.114 | 0.267 | 0.197 | 0.086 | 0.184 | 0.095 | 0.172 | 0.068 | 0.101 | 0.047 | 0.054 | 0.233 |
| Mixer outlet_CC CH4 | 0.221 | 0.116 | 0.241 | 0.193 | 0.071 | 0.167 | 0.083 | 0.156 | 0.059 | 0.086 | 0.037 | 0.043 | 0.225 |
| Mixer outlet_CC Benzene | 0.030 | 0.001 | 0.032 | 0.008 | 0.017 | 0.012 | 0.013 | 0.012 | 0.011 | 0.018 | 0.006 | 0.006 | 0.012 |
| Mixer outlet_CC Toluene | 0.006 | 0.001 | 0.007 | 0.004 | 0.002 | 0.005 | 0.001 | 0.005 | 0.001 | 0.002 | 0.005 | 0.006 | 0.004 |
| Mixer outlet_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| FUR IN Molar Flow | 0.332 | 0.174 | 0.361 | 0.265 | 0.167 | 0.326 | 0.166 | 0.302 | 0.116 | 0.186 | 0.085 | 0.097 | 0.324 |
| FUR IN P | 0.360 | 0.190 | 0.391 | 0.296 | 0.159 | 0.177 | 0.135 | 0.168 | 0.108 | 0.176 | 0.028 | 0.034 | 0.356 |
| FUR IN Temp | 0.495 | 0.222 | 0.538 | 0.379 | 0.163 | 0.305 | 0.176 | 0.284 | 0.130 | 0.185 | 0.088 | 0.100 | 0.453 |
| FUR IN_CC H2 | 0.245 | 0.114 | 0.267 | 0.197 | 0.086 | 0.184 | 0.095 | 0.172 | 0.068 | 0.100 | 0.047 | 0.054 | 0.233 |

| Table C1-2 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT14 | FT15 | FT16 | FT17 | FT18 | FT19 | FT20 | FT21 | FT22 | FT23 | FT24 | FT25 | FT26 |
| | IAE value | | | | | | | | | | | | |
| FUR IN_CCCH4 | 0.221 | 0.116 | 0.241 | 0.193 | 0.071 | 0.167 | 0.083 | 0.156 | 0.059 | 0.084 | 0.037 | 0.042 | 0.225 |
| FUR IN_CC Benzene | 0.030 | 0.001 | 0.032 | 0.008 | 0.017 | 0.012 | 0.013 | 0.012 | 0.011 | 0.018 | 0.006 | 0.006 | 0.012 |
| FUR IN_CC Toluene | 0.006 | 0.001 | 0.007 | 0.004 | 0.002 | 0.005 | 0.001 | 0.005 | 0.001 | 0.002 | 0.005 | 0.005 | 0.004 |
| FUR IN_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| RIN Molar Flow | 0.332 | 0.174 | 0.361 | 0.265 | 0.167 | 0.326 | 0.166 | 0.302 | 0.116 | 0.186 | 0.085 | 0.097 | 0.324 |
| RIN P | 0.390 | 0.239 | 0.424 | 0.346 | 0.190 | 0.239 | 0.164 | 0.225 | 0.127 | 0.210 | 0.029 | 0.035 | 0.417 |
| RIN Temp | 0.480 | 0.236 | 0.522 | 0.384 | 0.168 | 0.321 | 0.181 | 0.298 | 0.132 | 0.191 | 0.084 | 0.096 | 0.460 |
| RIN_CC H2 | 0.245 | 0.114 | 0.266 | 0.197 | 0.086 | 0.184 | 0.095 | 0.171 | 0.068 | 0.100 | 0.047 | 0.054 | 0.233 |
| RIN_CCCH4 | 0.221 | 0.116 | 0.241 | 0.193 | 0.071 | 0.167 | 0.083 | 0.155 | 0.059 | 0.084 | 0.037 | 0.042 | 0.225 |
| RIN_CC Benzene | 0.030 | 0.001 | 0.032 | 0.008 | 0.017 | 0.012 | 0.013 | 0.012 | 0.011 | 0.018 | 0.006 | 0.006 | 0.012 |
| RIN_CC Toluene | 0.006 | 0.001 | 0.007 | 0.004 | 0.002 | 0.005 | 0.001 | 0.005 | 0.001 | 0.002 | 0.005 | 0.005 | 0.004 |
| RIN_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| ROUT Molar Flow | 0.332 | 0.174 | 0.360 | 0.265 | 0.167 | 0.326 | 0.166 | 0.302 | 0.116 | 0.186 | 0.085 | 0.097 | 0.324 |
| ROUT P | 0.397 | 0.244 | 0.432 | 0.352 | 0.195 | 0.247 | 0.168 | 0.233 | 0.130 | 0.215 | 0.028 | 0.033 | 0.425 |
| ROUT Temp | 0.488 | 0.229 | 0.461 | 0.363 | 0.141 | 0.320 | 0.162 | 0.296 | 0.113 | 0.161 | 0.086 | 0.098 | 0.432 |
| ROUT_CC H2 | 0.263 | 0.125 | 0.286 | 0.215 | 0.092 | 0.207 | 0.104 | 0.193 | 0.073 | 0.108 | 0.056 | 0.063 | 0.253 |
| ROUT_CCCH4 | 0.250 | 0.131 | 0.272 | 0.218 | 0.081 | 0.198 | 0.096 | 0.184 | 0.067 | 0.098 | 0.048 | 0.054 | 0.255 |
| ROUT_CC Benzene | 0.038 | 0.007 | 0.041 | 0.018 | 0.019 | 0.028 | 0.017 | 0.027 | 0.013 | 0.021 | 0.012 | 0.014 | 0.024 |
| ROUT_CC Toluene | 0.035 | 0.017 | 0.039 | 0.029 | 0.012 | 0.026 | 0.014 | 0.024 | 0.010 | 0.014 | 0.006 | 0.007 | 0.034 |
| ROUT_CC Diphenyl | 0.010 | 0.004 | 0.011 | 0.007 | 0.004 | 0.007 | 0.004 | 0.007 | 0.003 | 0.005 | 0.002 | 0.003 | 0.009 |
| Quencher Molar Flow | 0.328 | 0.184 | 0.357 | 0.273 | 0.166 | 0.322 | 0.165 | 0.298 | 0.115 | 0.185 | 0.086 | 0.098 | 0.332 |
| Quencher P | 0.397 | 0.033 | 0.432 | 0.352 | 0.195 | 0.247 | 0.168 | 0.233 | 0.130 | 0.215 | 0.028 | 0.033 | 0.425 |
| Quencher Temp | 0.409 | 0.203 | 0.444 | 0.339 | 0.113 | 0.239 | 0.127 | 0.222 | 0.091 | 0.131 | 0.082 | 0.094 | 0.399 |

| Table C1-2 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT14 | FT15 | FT16 | FT17 | FT18 | FT19 | FT20 | FT21 | FT22 | FT23 | FT24 | FT25 | FT26 |
| | IAE value | | | | | | | | | | | | |
| Quencher_CC H2 | 0.256 | 0.120 | 0.279 | 0.207 | 0.090 | 0.203 | 0.101 | 0.189 | 0.072 | 0.105 | 0.054 | 0.061 | 0.245 |
| Quencher_CCCH4 | 0.236 | 0.128 | 0.257 | 0.210 | 0.076 | 0.186 | 0.090 | 0.173 | 0.063 | 0.090 | 0.045 | 0.052 | 0.245 |
| Quencher_CC Benzene | 0.056 | 0.011 | 0.060 | 0.029 | 0.025 | 0.043 | 0.024 | 0.041 | 0.018 | 0.028 | 0.014 | 0.016 | 0.036 |
| Quencher_CC Toluene | 0.051 | 0.025 | 0.056 | 0.042 | 0.018 | 0.037 | 0.020 | 0.035 | 0.014 | 0.021 | 0.009 | 0.011 | 0.050 |
| Quencher_CC Diphenyl | 0.016 | 0.007 | 0.018 | 0.011 | 0.007 | 0.011 | 0.007 | 0.010 | 0.005 | 0.007 | 0.003 | 0.004 | 0.014 |
| FEHE HOT-SIDE Molar Flow | 0.328 | 0.184 | 0.357 | 0.273 | 0.166 | 0.322 | 0.165 | 0.298 | 0.115 | 0.185 | 0.086 | 0.098 | 0.332 |
| FEHE HOT-SIDE P | 0.415 | 0.013 | 0.451 | 0.110 | 0.212 | 0.279 | 0.184 | 0.262 | 0.141 | 0.234 | 0.027 | 0.032 | 0.465 |
| FEHE HOT-SIDE Temp | 0.542 | 0.052 | 0.589 | 0.195 | 0.308 | 0.242 | 0.239 | 0.234 | 0.200 | 0.271 | 0.095 | 0.108 | 0.284 |
| FEHE HOT-SIDE_CC H2 | 0.256 | 0.120 | 0.280 | 0.207 | 0.090 | 0.203 | 0.102 | 0.189 | 0.072 | 0.105 | 0.054 | 0.061 | 0.245 |
| FEHE HOT-SIDE_CCCH4 | 0.236 | 0.128 | 0.259 | 0.210 | 0.076 | 0.186 | 0.092 | 0.172 | 0.063 | 0.090 | 0.045 | 0.052 | 0.245 |
| FEHE HOT-SIDE_CC Benzene | 0.056 | 0.011 | 0.061 | 0.029 | 0.025 | 0.043 | 0.025 | 0.041 | 0.018 | 0.028 | 0.014 | 0.016 | 0.036 |
| FEHE HOT-SIDE_CC Toluene | 0.051 | 0.025 | 0.056 | 0.042 | 0.018 | 0.037 | 0.020 | 0.035 | 0.014 | 0.021 | 0.009 | 0.011 | 0.050 |
| FEHE HOT-SIDE_CC Diphenyl | 0.016 | 0.007 | 0.018 | 0.011 | 0.007 | 0.011 | 0.007 | 0.010 | 0.005 | 0.007 | 0.003 | 0.004 | 0.014 |
| SEP INLET Molar Flow | 0.328 | 0.184 | 0.356 | 0.273 | 0.166 | 0.322 | 0.165 | 0.298 | 0.115 | 0.185 | 0.086 | 0.098 | 0.332 |
| SEP INLET P | 0.415 | 0.012 | 0.451 | 0.111 | 0.212 | 0.280 | 0.184 | 0.263 | 0.141 | 0.234 | 0.027 | 0.032 | 0.163 |
| SEP INLET Temp | 0.500 | 0.045 | 0.544 | 0.093 | 0.287 | 0.186 | 0.214 | 0.182 | 0.184 | 0.316 | 0.096 | 0.110 | 0.157 |
| SEP INLET_CC H2 | 0.256 | 0.120 | 0.279 | 0.207 | 0.090 | 0.203 | 0.101 | 0.188 | 0.072 | 0.106 | 0.054 | 0.061 | 0.244 |
| SEP INLET_CCCH4 | 0.236 | 0.128 | 0.256 | 0.210 | 0.076 | 0.186 | 0.090 | 0.172 | 0.063 | 0.092 | 0.045 | 0.052 | 0.245 |
| SEP INLET_CC Benzene | 0.055 | 0.011 | 0.060 | 0.029 | 0.025 | 0.043 | 0.024 | 0.040 | 0.018 | 0.029 | 0.014 | 0.016 | 0.036 |
| SEP INLET_CC Toluene | 0.051 | 0.025 | 0.056 | 0.042 | 0.018 | 0.037 | 0.020 | 0.035 | 0.014 | 0.021 | 0.009 | 0.011 | 0.050 |
| SEP INLET_CC Diphenyl | 0.016 | 0.007 | 0.018 | 0.011 | 0.007 | 0.011 | 0.007 | 0.010 | 0.005 | 0.007 | 0.003 | 0.004 | 0.014 |
| SEP GAS Molar Flow | 0.277 | 0.156 | 0.301 | 0.231 | 0.142 | 0.301 | 0.145 | 0.277 | 0.099 | 0.158 | 0.082 | 0.094 | 0.281 |
| SEP GAS P | 0.415 | 0.012 | 0.451 | 0.111 | 0.212 | 0.280 | 0.184 | 0.263 | 0.141 | 0.234 | 0.027 | 0.032 | 0.163 |

| Table C1-2 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT14 | FT15 | FT16 | FT17 | FT18 | FT19 | FT20 | FT21 | FT22 | FT23 | FT24 | FT25 | FT26 |
| | IAE value | | | | | | | | | | | | |
| SEP GAS Temp | 0.500 | 0.045 | 0.543 | 0.093 | 0.287 | 0.186 | 0.214 | 0.182 | 0.184 | 0.316 | 0.096 | 0.109 | 0.157 |
| SEP GAS_CC H2 | 0.288 | 0.135 | 0.313 | 0.233 | 0.101 | 0.222 | 0.113 | 0.207 | 0.081 | 0.118 | 0.059 | 0.067 | 0.275 |
| SEP GAS_CCCH4 | 0.253 | 0.137 | 0.276 | 0.226 | 0.081 | 0.209 | 0.098 | 0.194 | 0.068 | 0.097 | 0.052 | 0.059 | 0.263 |
| SEP GAS_CC Benzene | 0.035 | 0.001 | 0.038 | 0.009 | 0.020 | 0.014 | 0.015 | 0.014 | 0.013 | 0.021 | 0.007 | 0.008 | 0.014 |
| SEP GAS_CC Toluene | 0.001 | 0.001 | 0.001 | 0.001 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 |
| SEP GAS_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| SEP LIQ Molar Flow | 0.051 | 0.028 | 0.056 | 0.042 | 0.024 | 0.021 | 0.020 | 0.020 | 0.017 | 0.026 | 0.004 | 0.005 | 0.051 |
| SEP LIQ P | 0.415 | 0.012 | 0.451 | 0.111 | 0.212 | 0.280 | 0.184 | 0.263 | 0.141 | 0.234 | 0.027 | 0.032 | 0.163 |
| SEP LIQ Temp | 0.500 | 0.045 | 0.543 | 0.093 | 0.287 | 0.186 | 0.214 | 0.182 | 0.184 | 0.316 | 0.096 | 0.109 | 0.157 |
| SEP LIQ_CC H2 | 0.001 | 0.002 | 0.001 | 0.002 | 0.000 | 0.002 | 0.000 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.003 |
| SEP LIQ_CCCH4 | 0.002 | 0.010 | 0.002 | 0.012 | 0.004 | 0.009 | 0.001 | 0.008 | 0.002 | 0.005 | 0.001 | 0.001 | 0.012 |
| SEP LIQ_CC Benzene | 0.335 | 0.166 | 0.365 | 0.280 | 0.113 | 0.256 | 0.130 | 0.239 | 0.092 | 0.136 | 0.061 | 0.069 | 0.329 |
| SEP LIQ_CC Toluene | 0.502 | 0.242 | 0.546 | 0.407 | 0.178 | 0.374 | 0.196 | 0.348 | 0.141 | 0.206 | 0.094 | 0.107 | 0.482 |
| SEP LIQ_CC Diphenyl | 0.168 | 0.069 | 0.182 | 0.118 | 0.069 | 0.111 | 0.068 | 0.103 | 0.050 | 0.076 | 0.034 | 0.039 | 0.143 |
| COMP INLET Molar Flow | 0.263 | 0.147 | 0.286 | 0.218 | 0.136 | 0.300 | 0.140 | 0.277 | 0.094 | 0.152 | 0.089 | 0.102 | 0.266 |
| COMP INLET P | 0.415 | 0.012 | 0.451 | 0.111 | 0.212 | 0.074 | 0.184 | 0.263 | 0.141 | 0.234 | 0.027 | 0.032 | 0.163 |
| COMP INLET Temp | 0.499 | 0.045 | 0.543 | 0.093 | 0.287 | 0.167 | 0.278 | 0.182 | 0.184 | 0.316 | 0.096 | 0.109 | 0.157 |
| COMP INLET_CC H2 | 0.288 | 0.135 | 0.313 | 0.233 | 0.101 | 0.222 | 0.113 | 0.207 | 0.081 | 0.119 | 0.059 | 0.067 | 0.275 |
| COMP INLET_CCCH4 | 0.253 | 0.137 | 0.276 | 0.225 | 0.081 | 0.209 | 0.098 | 0.194 | 0.068 | 0.099 | 0.052 | 0.059 | 0.262 |
| COMP INLET_CC Benzene | 0.035 | 0.001 | 0.038 | 0.009 | 0.020 | 0.014 | 0.015 | 0.014 | 0.013 | 0.021 | 0.007 | 0.008 | 0.014 |
| COMP INLET_CC Toluene | 0.001 | 0.001 | 0.001 | 0.001 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 |
| COMP INLET_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| GAS RECYCLE Molar Flow | 0.263 | 0.147 | 0.286 | 0.218 | 0.136 | 0.300 | 0.140 | 0.277 | 0.094 | 0.152 | 0.089 | 0.102 | 0.266 |

| Table C1-2 (Continue) | Key process variables | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| process variables | FT14 | FT15 | FT16 | FT17 | FT18 | FT19 | FT20 | FT21 | FT22 | FT23 | FT24 | FT25 | FT26 |
| | IAE value | | | | | | | | | | | | |
| GAS RECYCLE P | 0.370 | 0.147 | 0.402 | 0.258 | 0.164 | 0.144 | 0.139 | 0.139 | 0.117 | 0.183 | 0.024 | 0.029 | 0.315 |
| GAS RECYCLE Temp | 0.500 | 0.036 | 0.543 | 0.101 | 0.287 | 0.178 | 0.279 | 0.180 | 0.248 | 0.316 | 0.098 | 0.112 | 0.165 |
| GAS RECYCLE_CC H2 | 0.288 | 0.135 | 0.313 | 0.233 | 0.101 | 0.222 | 0.113 | 0.207 | 0.081 | 0.119 | 0.059 | 0.067 | 0.275 |
| GAS RECYCLE_CCCH4 | 0.253 | 0.136 | 0.276 | 0.225 | 0.081 | 0.209 | 0.098 | 0.194 | 0.068 | 0.099 | 0.052 | 0.059 | 0.262 |
| GAS RECYCLE_CC Benzene | 0.035 | 0.001 | 0.038 | 0.009 | 0.020 | 0.014 | 0.015 | 0.014 | 0.013 | 0.021 | 0.007 | 0.008 | 0.014 |
| GAS RECYCLE_CC Toluene | 0.001 | 0.001 | 0.001 | 0.001 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 |
| GAS RECYCLE_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| PURGE Molar Flow | 0.014 | 0.009 | 0.015 | 0.013 | 0.006 | 0.006 | 0.004 | 0.005 | 0.004 | 0.006 | 0.008 | 0.009 | 0.016 |
| PURGE P | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.277 | 0.000 |
| PURGE Temp | 0.496 | 0.046 | 0.538 | 0.090 | 0.285 | 0.182 | 0.213 | 0.179 | 0.183 | 0.314 | 0.096 | 0.107 | 0.153 |
| PURGE_CC H2 | 0.288 | 0.135 | 0.313 | 0.233 | 0.101 | 0.222 | 0.113 | 0.207 | 0.081 | 0.120 | 0.059 | 0.067 | 0.275 |
| PURGE_CCCH4 | 0.253 | 0.137 | 0.276 | 0.225 | 0.081 | 0.209 | 0.098 | 0.194 | 0.068 | 0.101 | 0.052 | 0.059 | 0.262 |
| PURGE_CC Benzene | 0.035 | 0.001 | 0.038 | 0.009 | 0.020 | 0.014 | 0.015 | 0.014 | 0.013 | 0.021 | 0.007 | 0.008 | 0.014 |
| PURGE_CC Toluene | 0.001 | 0.001 | 0.001 | 0.001 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 |
| PURGE_CC Diphenyl | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| TOL RECYCLE Molar Flow | 0.001 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| TOL RECYCLE P | 0.370 | 0.147 | 0.402 | 0.258 | 0.164 | 0.144 | 0.139 | 0.139 | 0.117 | 0.183 | 0.024 | 0.029 | 0.315 |
| TOL RECYCLE Temp | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| sum IAE | 21.034 | 7.637 | 22.807 | 13.507 | 9.324 | 13.961 | 8.949 | 13.300 | 6.735 | 10.435 | 3.734 | 4.551 | 16.964 |

Note:

FT1 = Fresh toluene feed flowrate

FT2 = Pressure of fresh feed toluene stream

FT3 = Temperature of fresh feed toluene stream

FT4 = Fresh hydrogen feed flowrate

FT5 = Pressure of fresh feed hydrogen stream

FT6 = Temperature of fresh feed hydrogen stream

FT7 = Mixer outlet pressure

FT8 = Mixer outlet temperature

FT9 = Furnace inlet pressure

FT10 = Furnace inlet temperature

FT11 = Reactor inlet pressure

FT12 = Reactor inlet temperature

FT13 = Reactor outlet pressure

FT14 = Reactor outlet temperature

FT15 = Quencher outlet pressure

FT16 = Quencher outlet temperature

FT17 = FEHE hot-side outlet pressure

FT18 = FEHE hot-side outlet temperature

FT19 = Compressor inlet pressure

FT20 = Compressor inlet temperature

FT21 = Gas recycle pressure

FT22 = Gas recycle temperature

FT23 = Separator inlet temperature

FT24 = Purge flowrate

FT25 = Purge pressure

FT26 = Separator pressure

# APPENDIX D

## HDA process flowsheet with controller installed

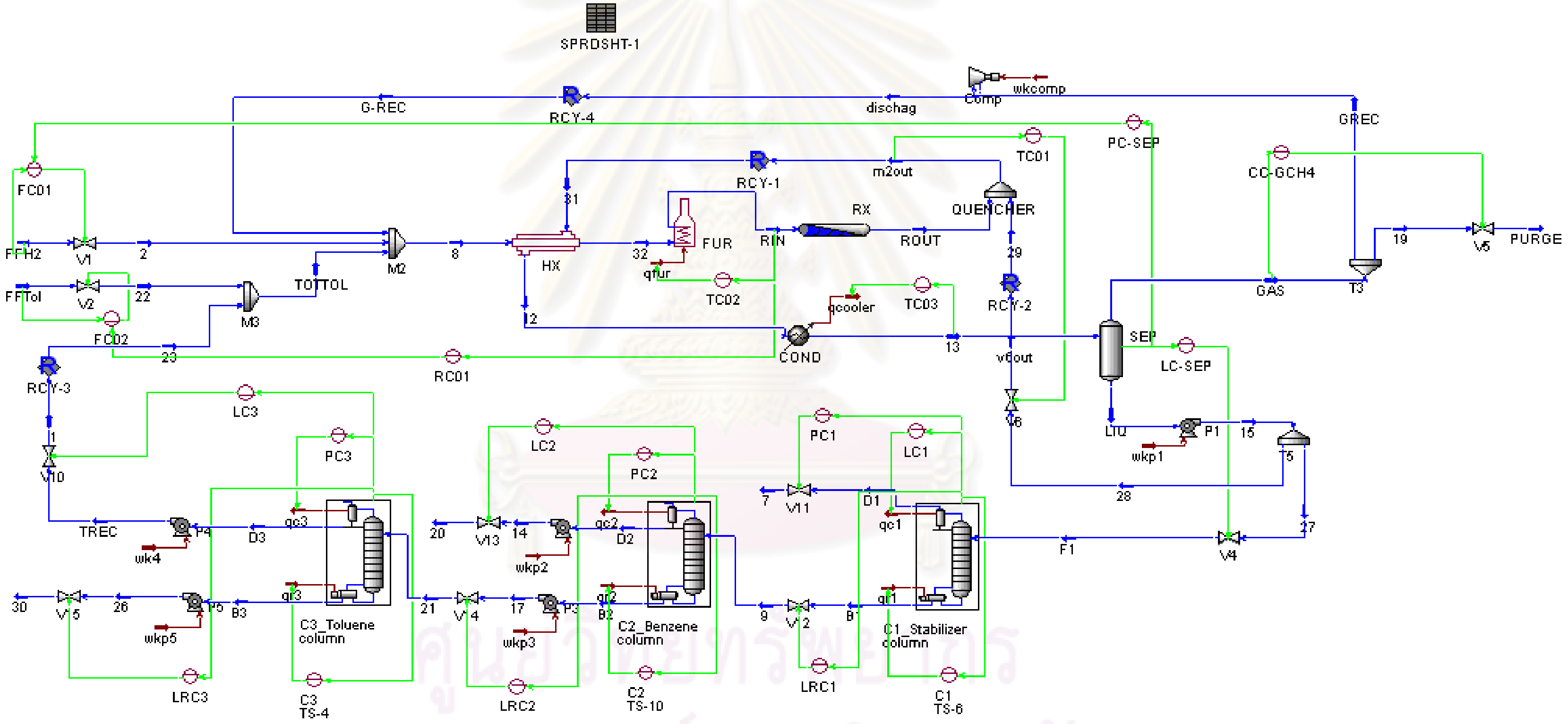


Figure D.1 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed control structure 1 (CS1)

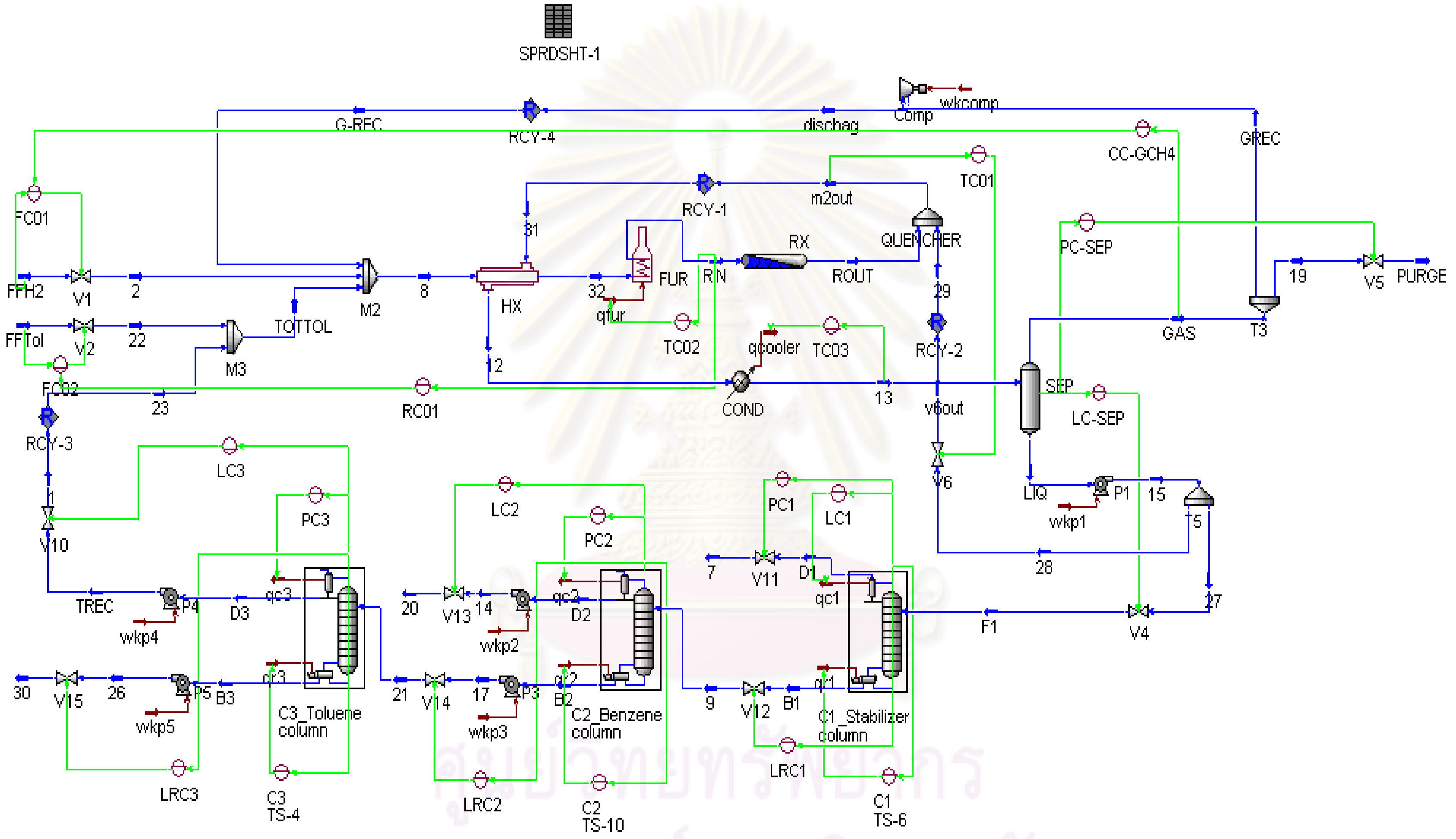


Figure D.2 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed control structure 2 (CS2)

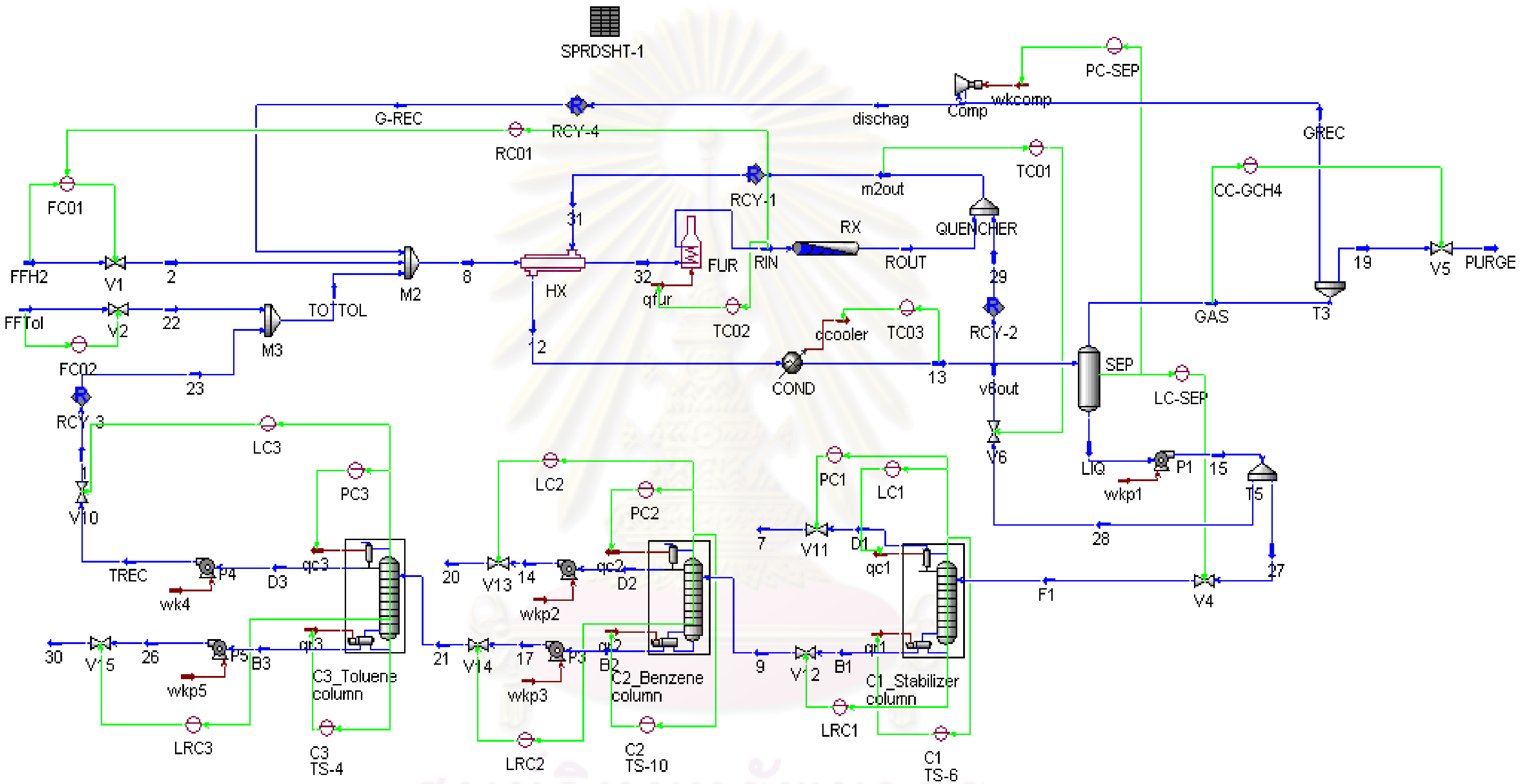


**Figure D.3** The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed control structure 3 (CS3)

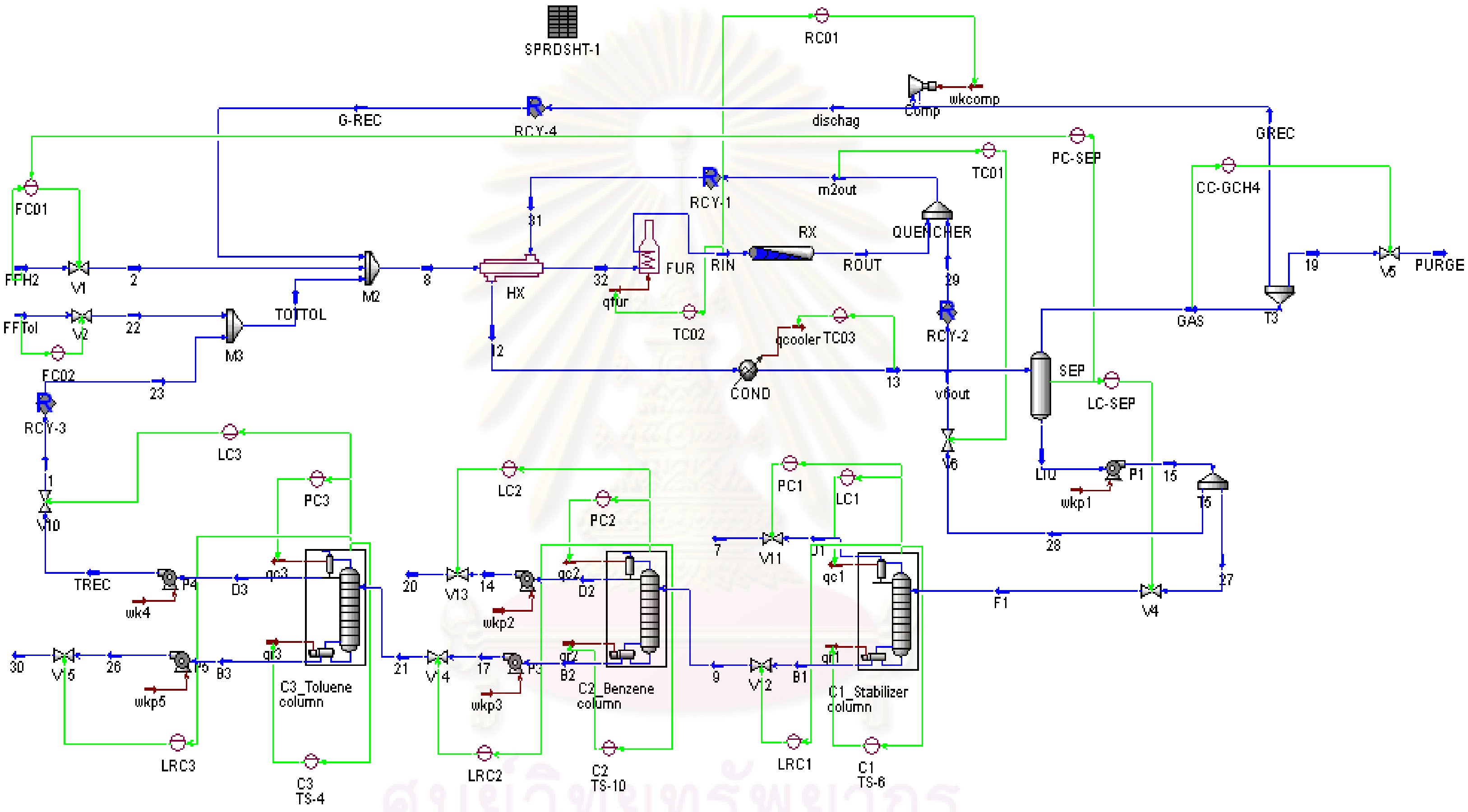


Figure D.4 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed control structure 4 (CS4)

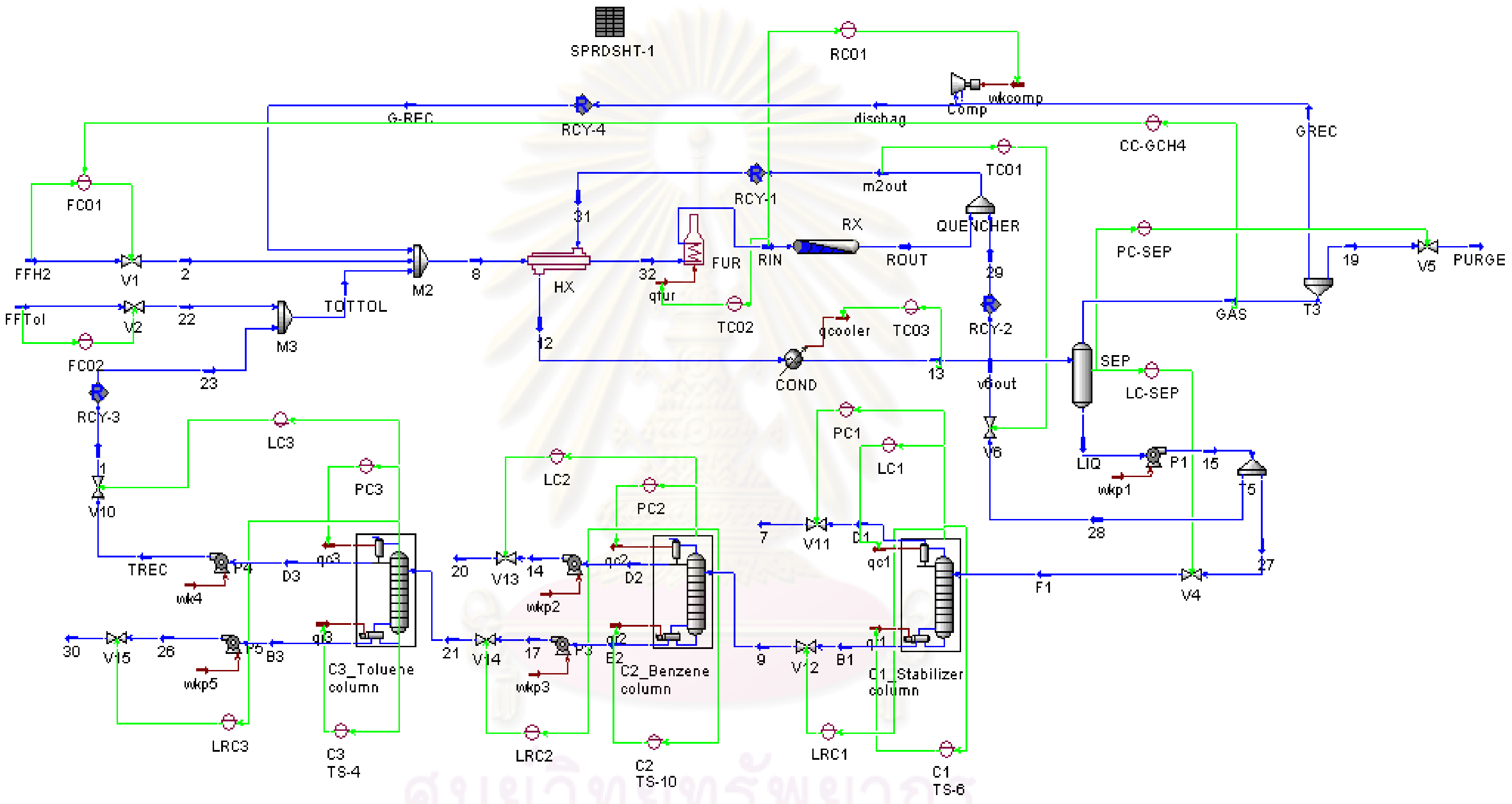


Figure D.5 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed control structure 5 (CS5)

Table D.1 Steady-state controlled variables selected by various authors (Reaction section)

| Controlled variable (Reaction section) | authors | | | | | |
|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4/1* | 4/2* | 4/3* |
| Fresh toluene feed rate (FFTOL) | | X | X | X | X | X |
| Fresh gas hydrogen feed rate (FFH2) | | X | | X | X | X |
| Recycle gas methane mole fraction | X | | | | | |
| Reactor inlet pressure (Prin) | | X | X | | | X |
| Compressor power | X | | | | | |
| Total toluene flow rate to the reaction section | X | | | | | |
| Mixer outlet methane mole fraction (Xmet,mix) | | X | | | X | X |
| Reactor inlet temperature (Trin) | X | X | X | X | X | X |
| Reactor outlet temperature (Trout) | | | X | | | |
| Separator temperature | X | X | X | X | X | X |
| Separator pressure | X | | | X | X | |
| Separator overhead vapor methane mole fraction | | | X | X | | |
| Hydrogen to aromatic ratio at reactor inlet (rH2) | | X | X | X | X | X |
| Quencher outlet temperature | X | X | X | X | X | X |
| Quencher outlet toluene mole fraction | | X | | | | |

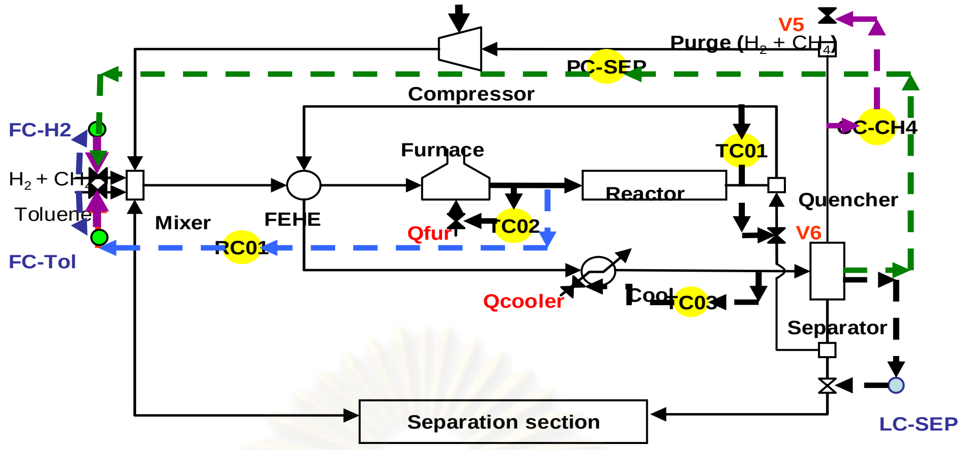
Note: 1=Luyben (1998), 2=Araujo et al.(2006) 3= Kiatpiriya C. (reaction section only, 2007), 4*= This work (4/1 = SET1 (Set of CVs) 4/2 = SET2 and 4/3=SET3)

Table D.2 Steady-state controlled variables selected by various authors (Separation section)

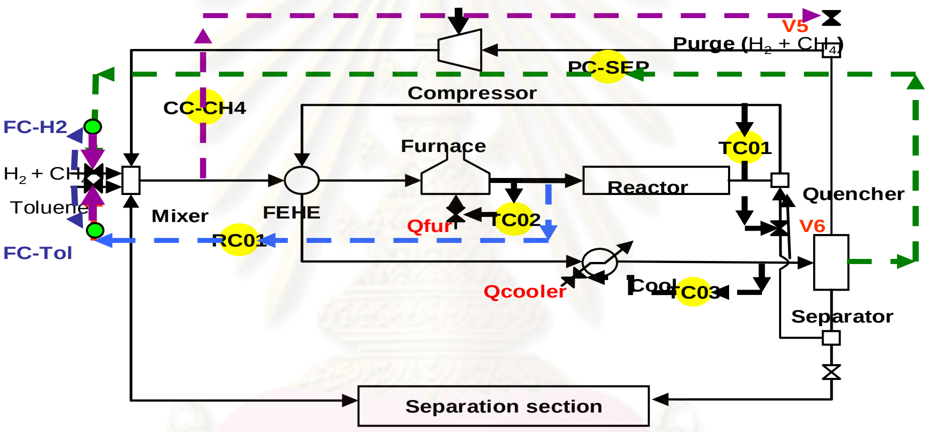
| Controlled variable (Separation section) | authors | | | | | |
|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4/1* | 4/2* | 4/3* |
| Benzene mole fraction in stabilizer column distillate | | X | | | | |
| Methane mole fraction in stabilizer column bottoms | | X | | | | |
| Benzene mole fraction in benzene column distillate | | X | | | | |
| Benzene mole fraction in benzene column bottoms | | X | | | | |
| Toluene mole fraction in toluene column distillate | | X | | | | |
| Diphenyl mole fraction in toluene column distillate | | X | | | | |
| Temperature in stage 3 of the stabilizer column | | X | | | | |
| Temperature in stage 20 of the benzene column | | X | | | | |
| Temperature in stage 5 of the toluene column | | X | | | | |
| Temperature in stage 6 of the stabilizer column | X | | | | | |
| Temperature in stage 12 of the benzene column | X | | | | | |
| Average temperature of stage1-4 of the toluene column | X | | | | | |
| Temperature in stage 6 of the stabilizer column | | | | X | X | X |
| Temperature in stage 10 of the benzene column | | | | X | X | X |
| Temperature in stage 4 of the toluene column | | | | X | X | X |

Note: 1=Luyben (1998), 2=Araujo et al.(2006) 3= Kiatpiriya C. (reaction section only, 2007), 4*= This work (4/1 = SET1 (Set of CVs) 4/2 = SET2 and 4/3=SET3)

CS1-SET1



CS1-SET2



CS1-SET3

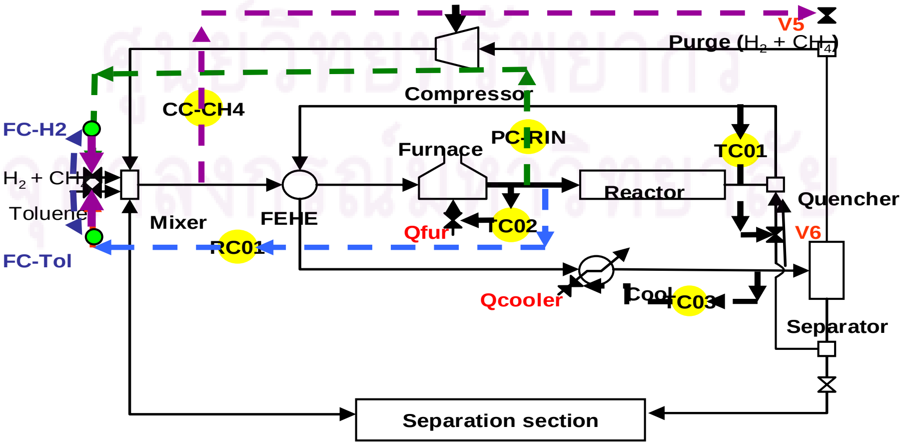
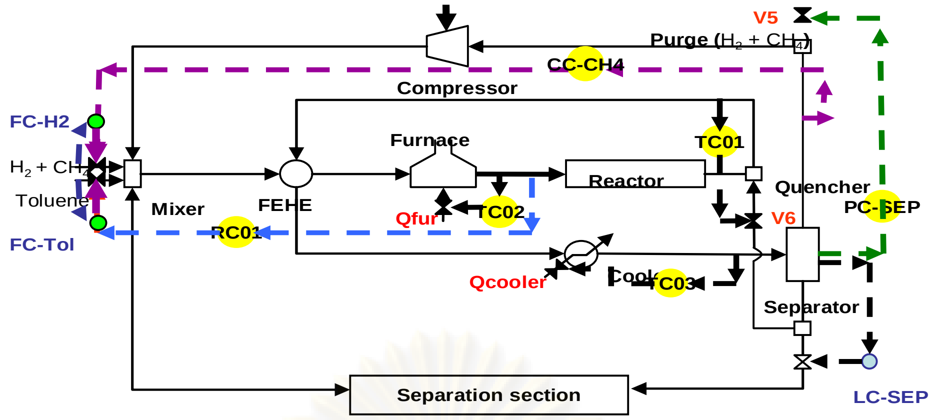
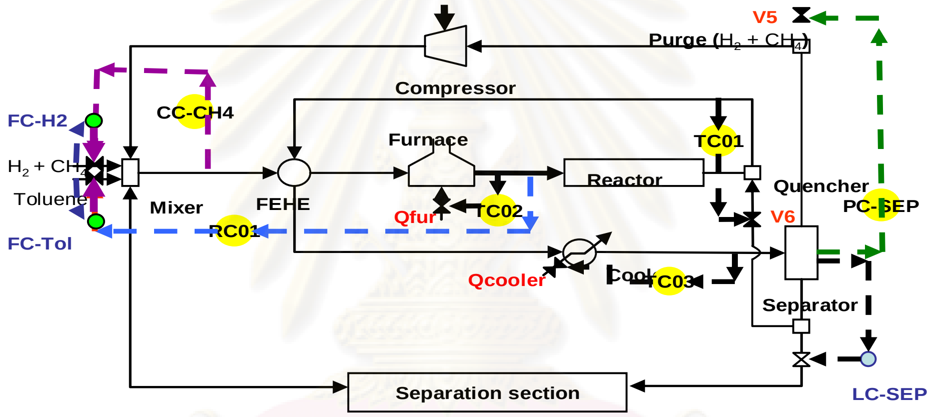


Figure D.6 The Flowsheet of HDA process (Reaction section) of CS1 compare between SET1, SET2 and SET3

CS2-SET1



CS2-SET2



CS2-SET3

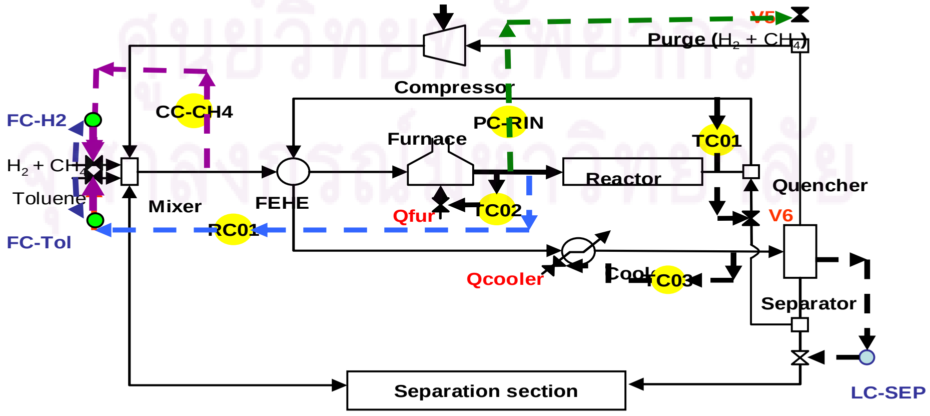
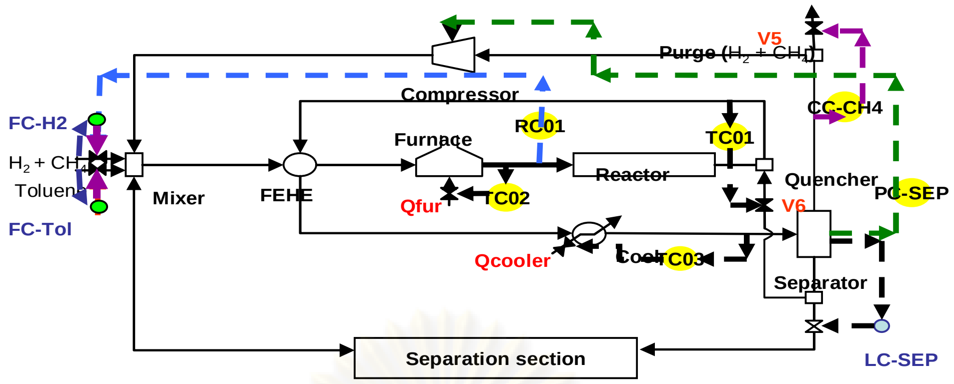
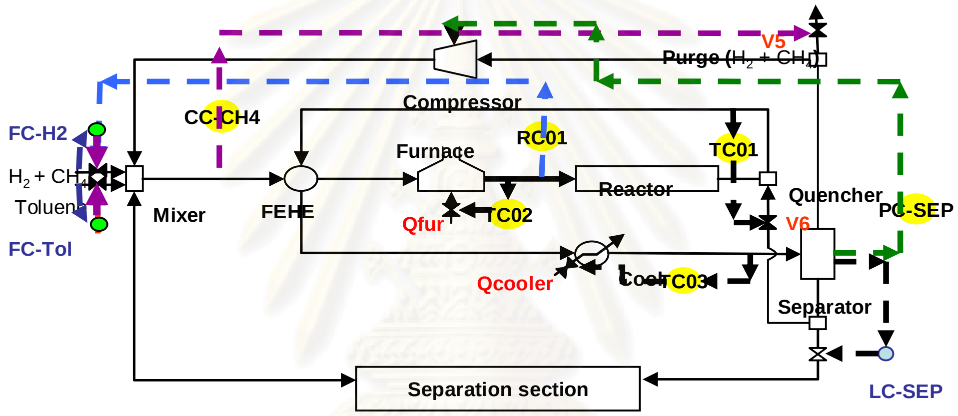


Figure D.7 The Flowsheet of HDA process (Reaction section) of CS2 compare between SET1, SET2 and SET3

CS3-SET1



CS3-SET2



CS3-SET3

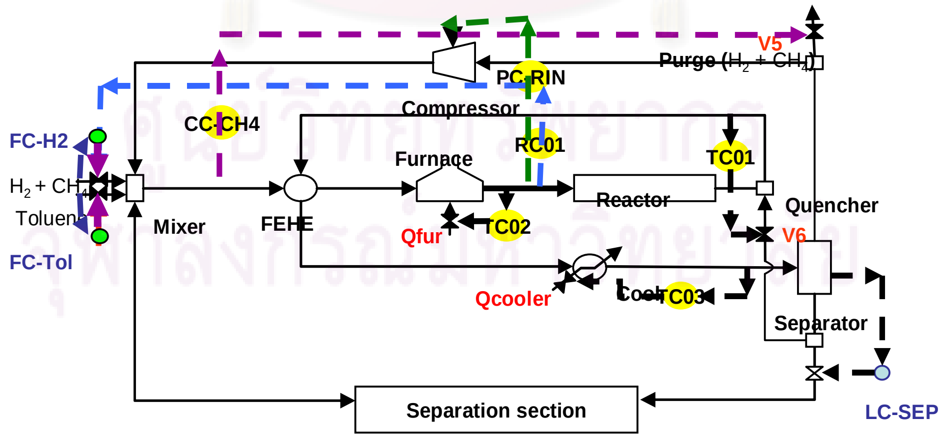
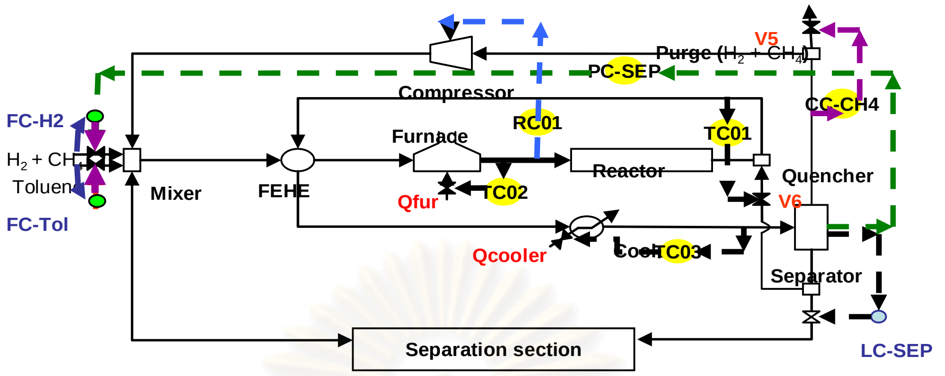
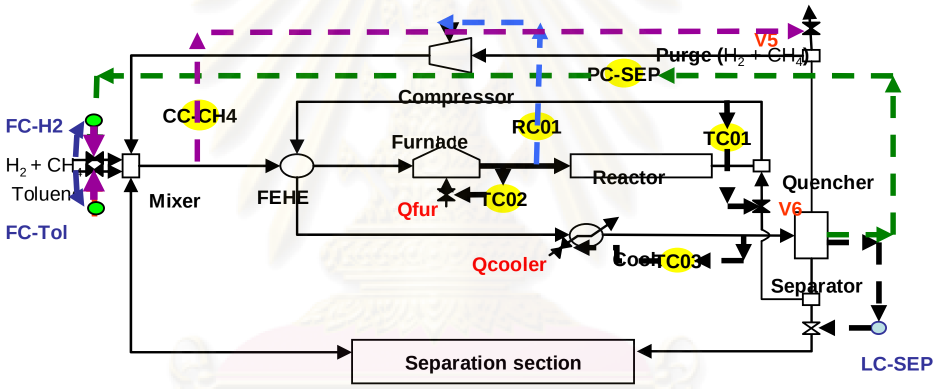


Figure D.8 The Flowsheet of HDA process (Reaction section) of CS3 compare between SET1, SET2 and SET3

CS4-SET1



CS4-SET2



CS4-SET3

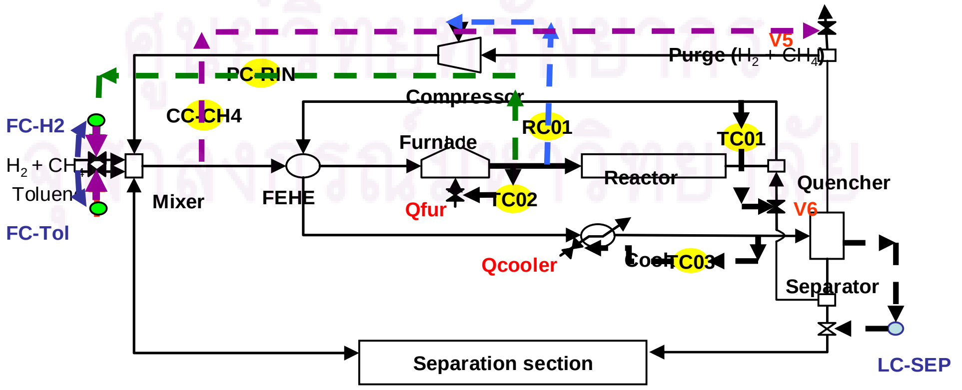
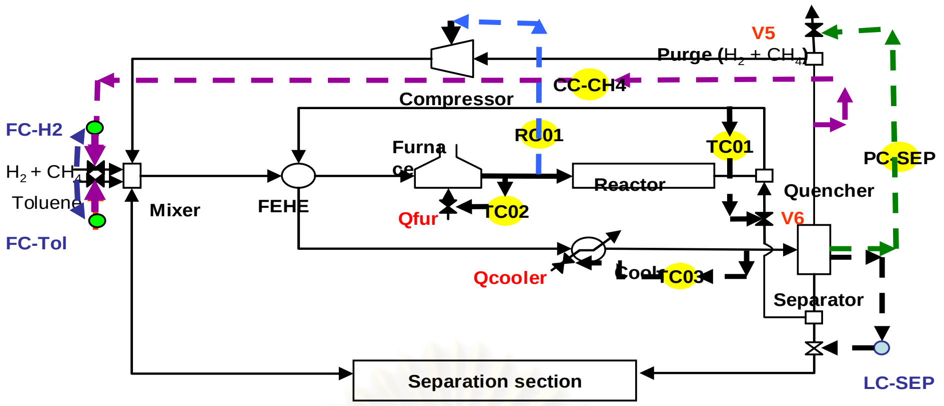
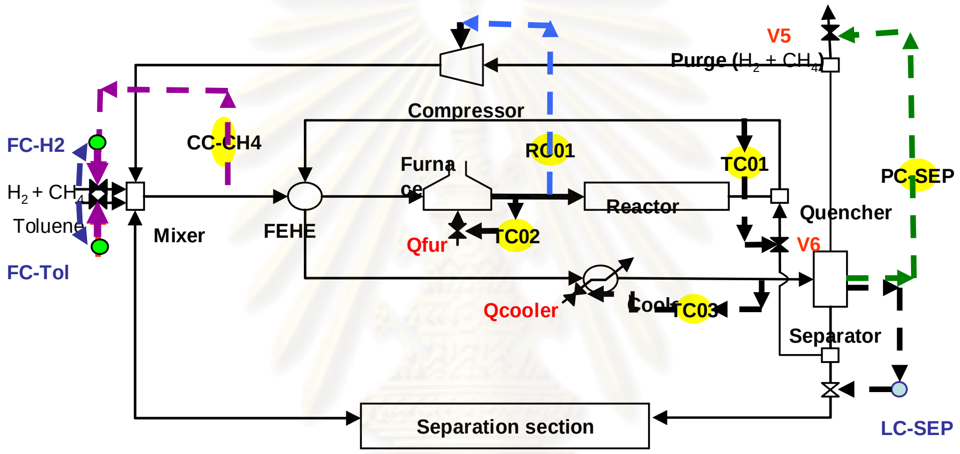


Figure D.9 The Flowsheet of HDA process (Reaction section) of CS4 compare between SET1, SET2 and SET3

CS5-SET1



CS5-SET2



CS5-SET3

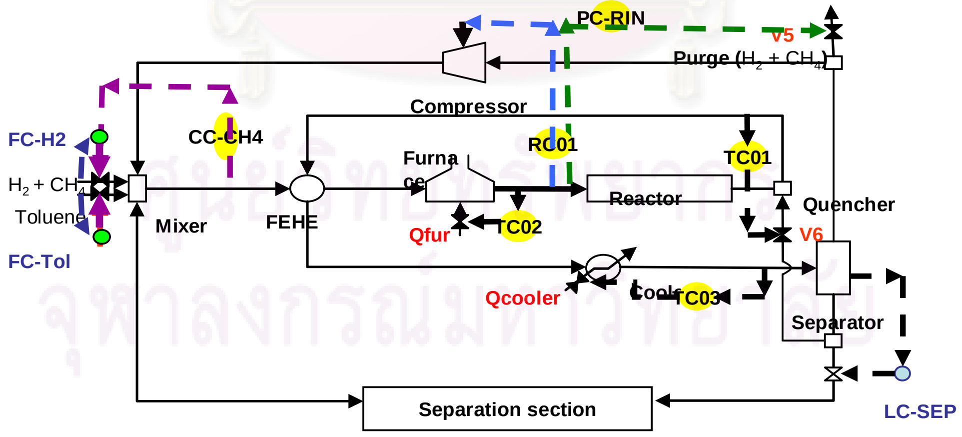
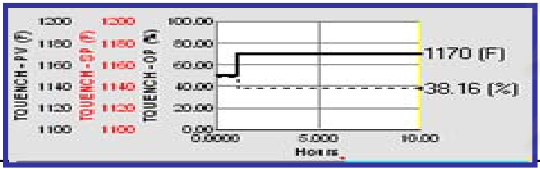
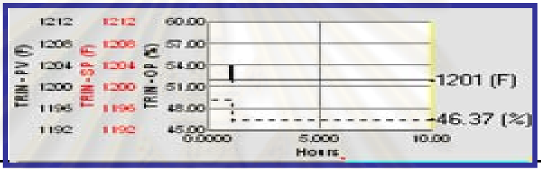
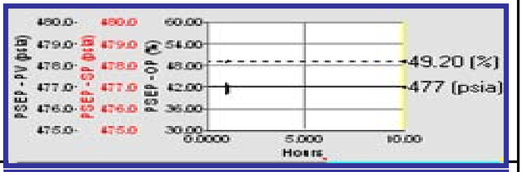
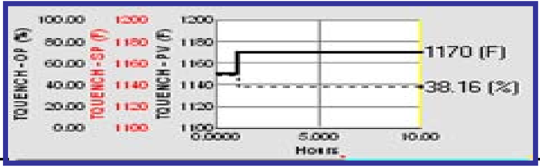
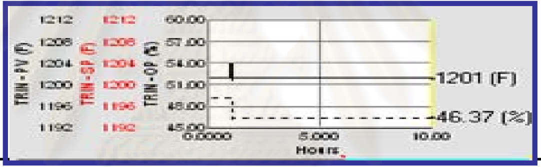
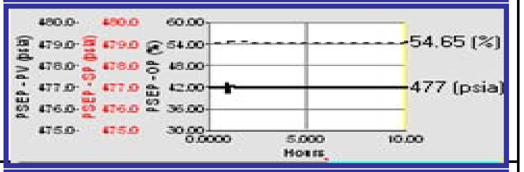
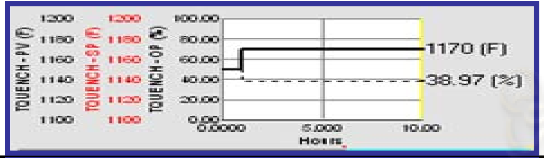
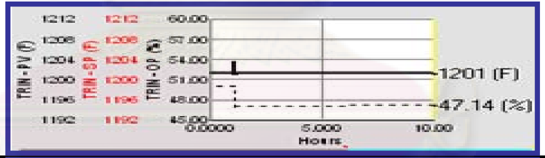
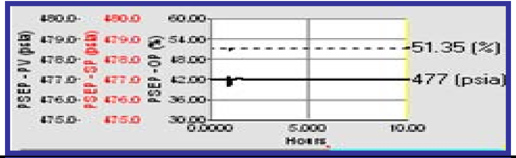
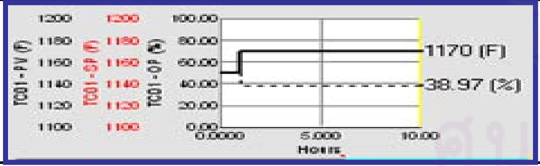
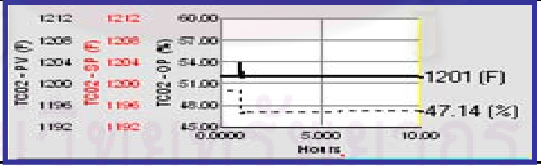
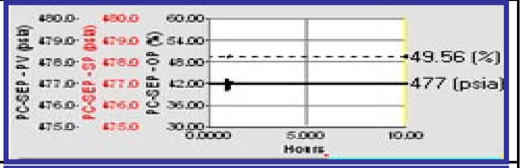
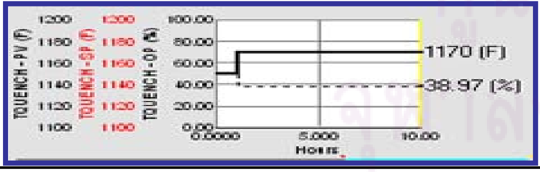
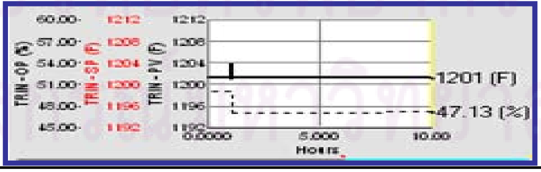
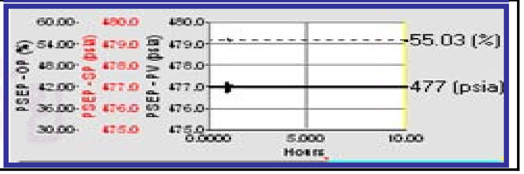
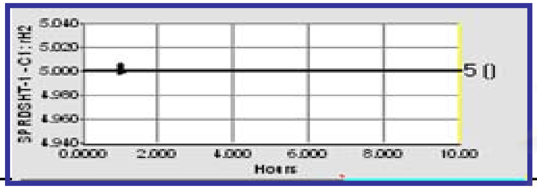
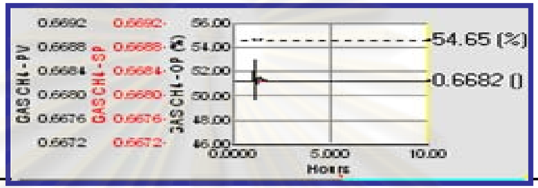
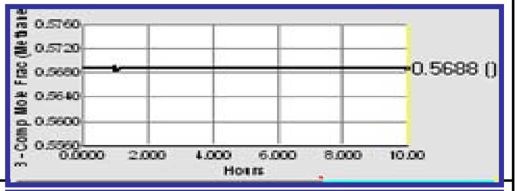
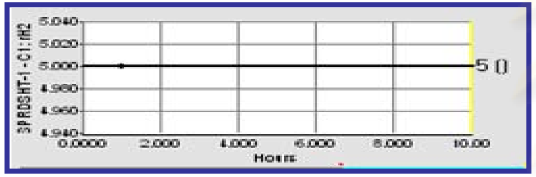
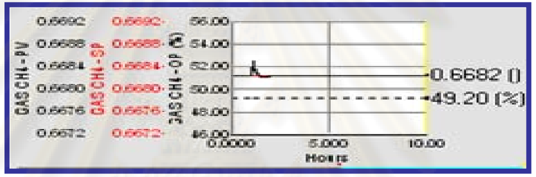
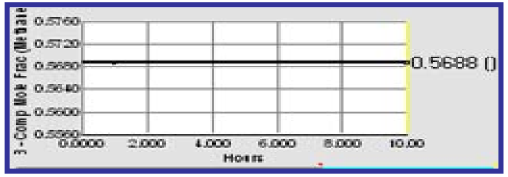
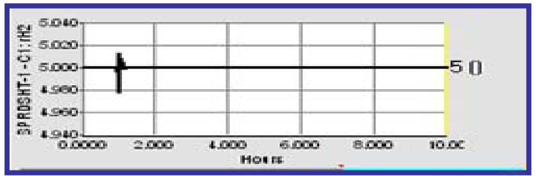
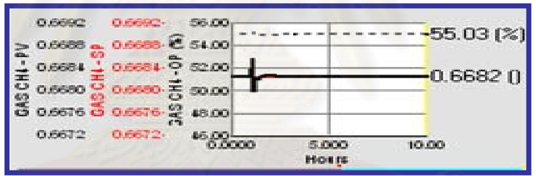
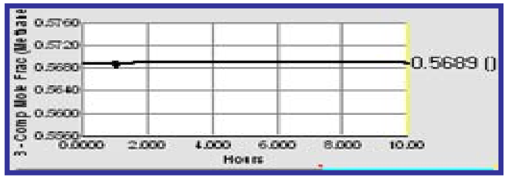
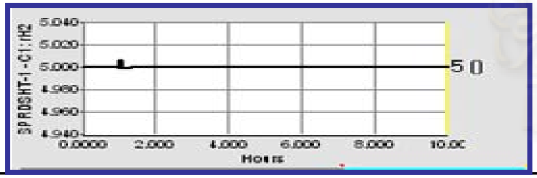
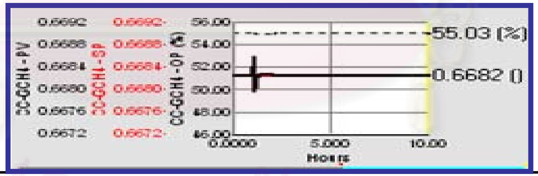
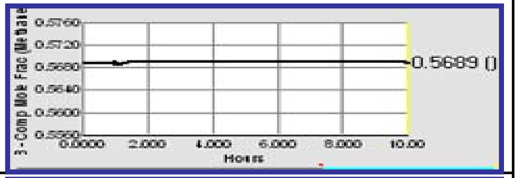
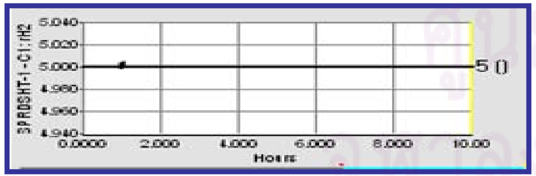
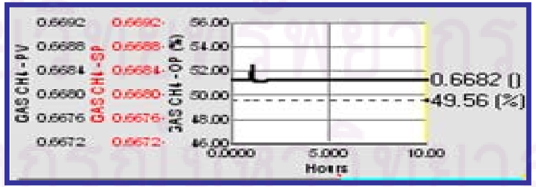
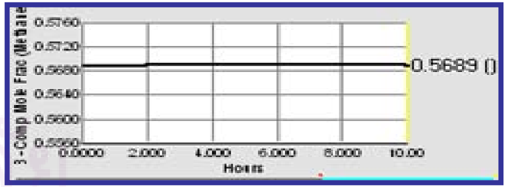


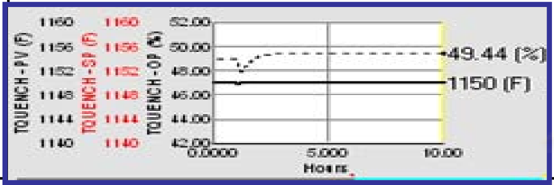
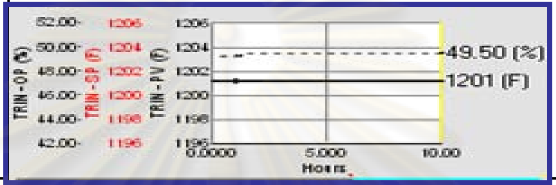
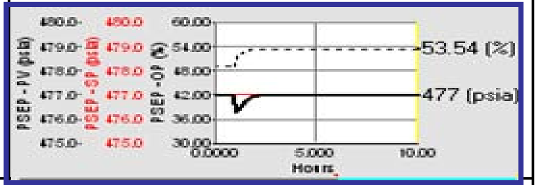
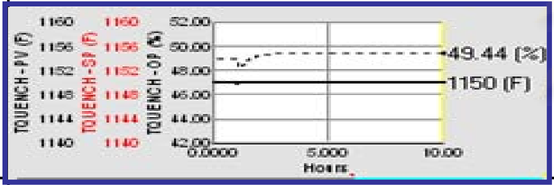
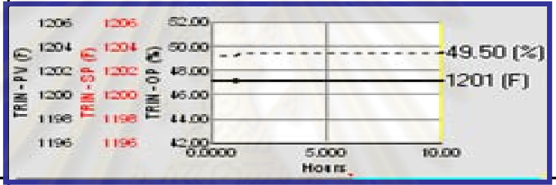
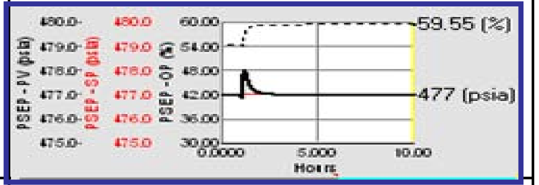
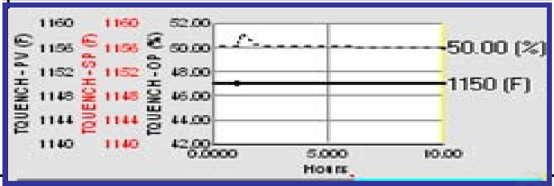
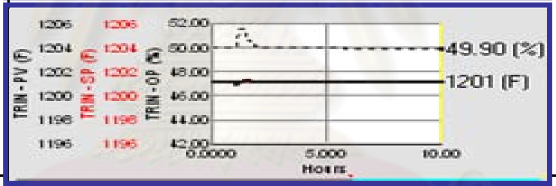
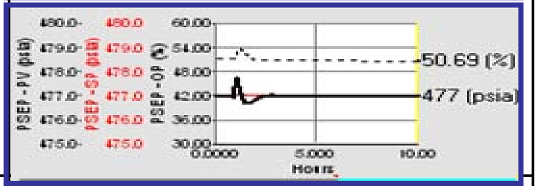
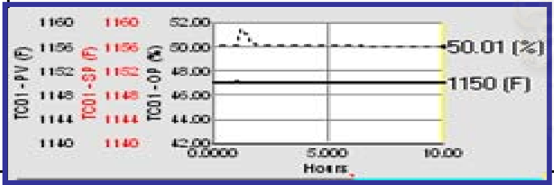
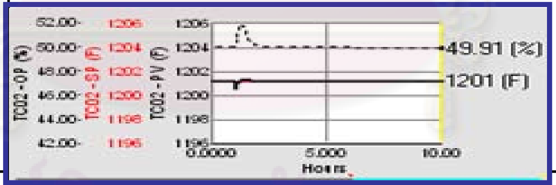
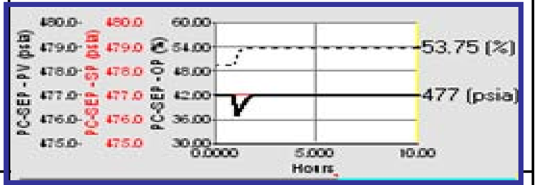
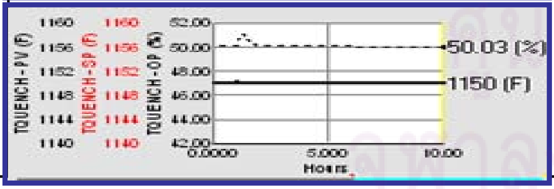
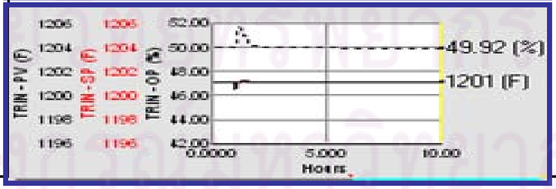
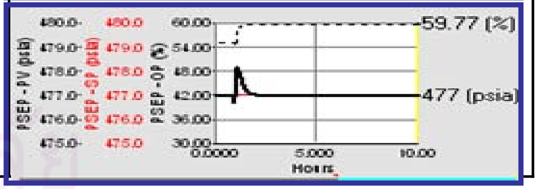
Figure D.10 The Flowsheet of HDA process (Reaction section) of CS5 compare between SET1, SET2 and SET3

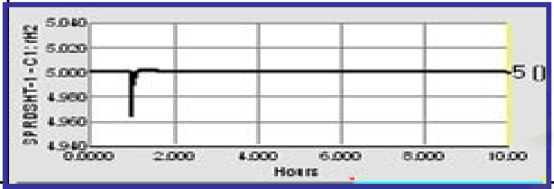
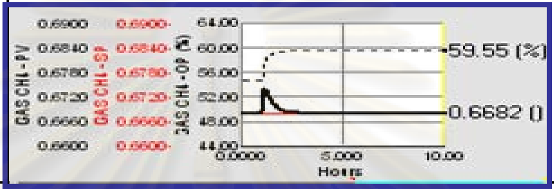
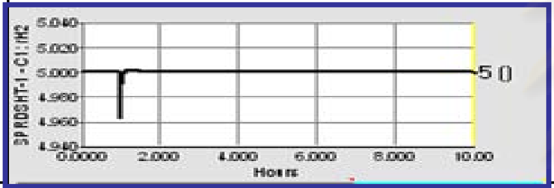
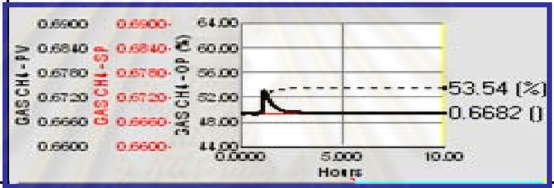
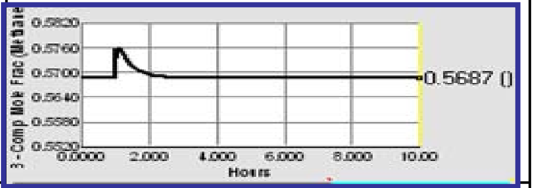
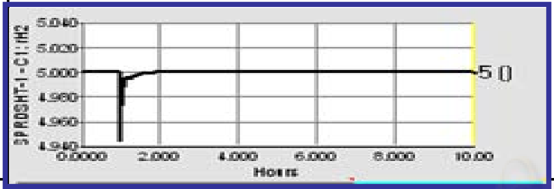
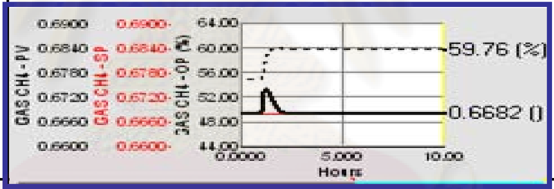
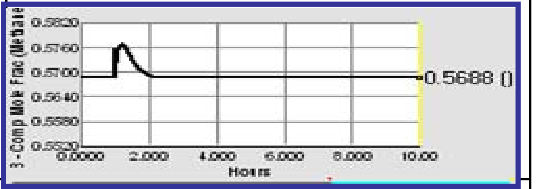
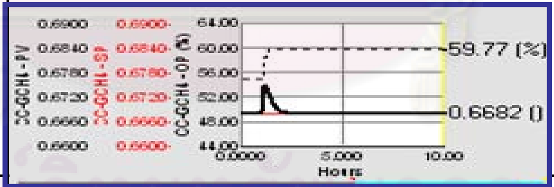
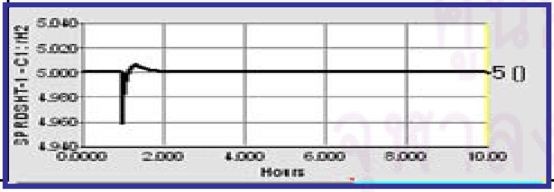
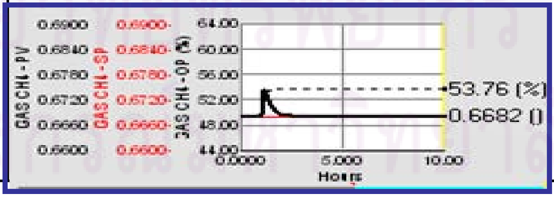
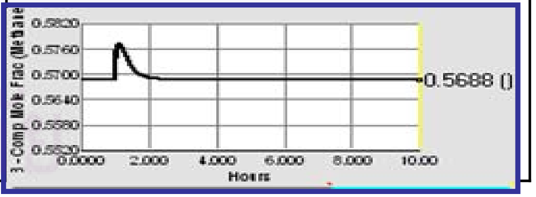
# APPENDIX E

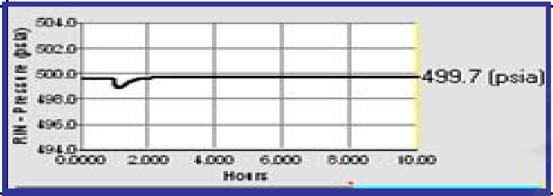
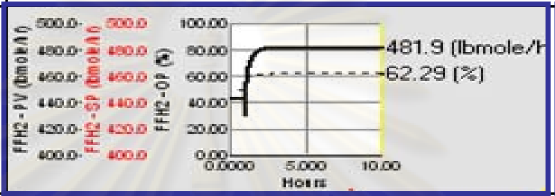
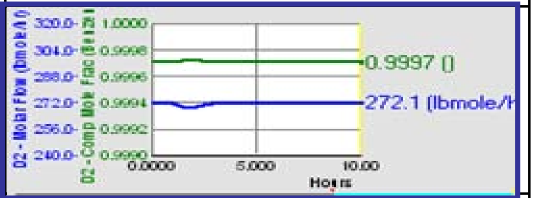
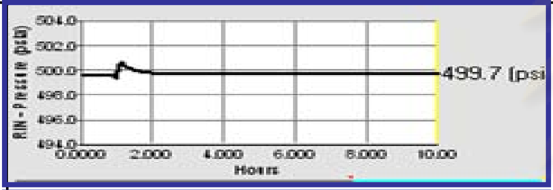
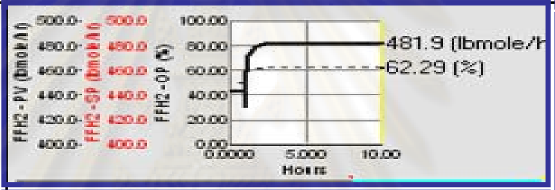
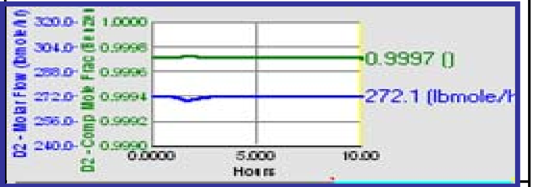
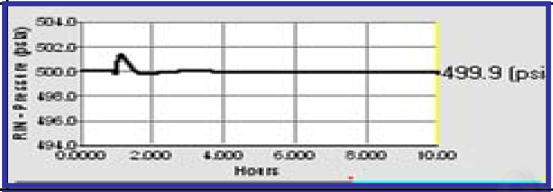
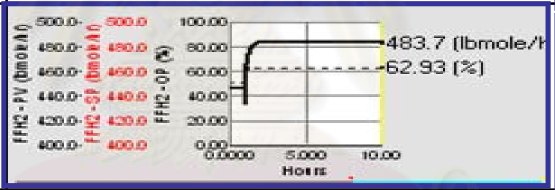
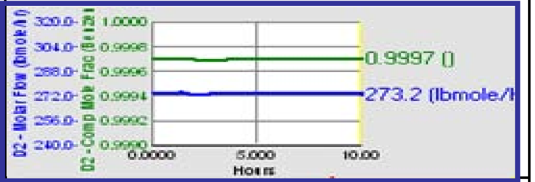
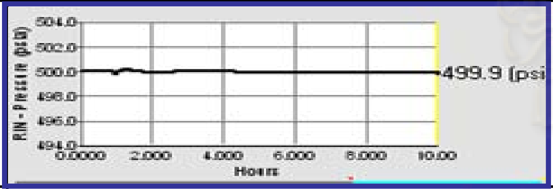
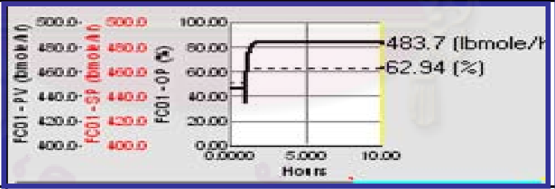
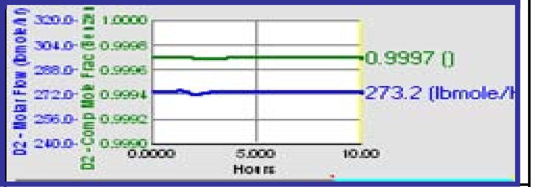
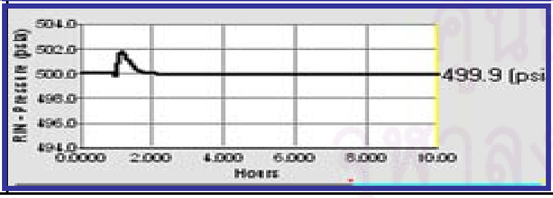
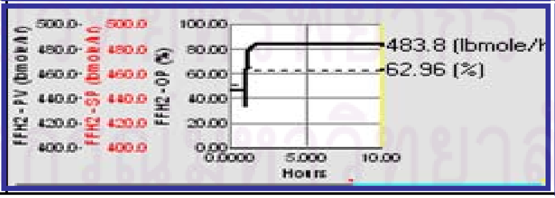
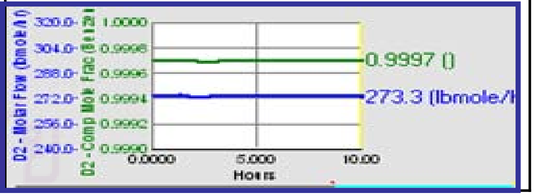
## Graph of dynamic response of SET1 (CS1-CS5)

| | SET1: D = +20 oF of quencher outlet temperature | | |
|---|---|---|---|
| | Tquen | Trin | Psep |
| CS1 |  |  |  |
| CS2 |  |  |  |
| CS3 |  |  |  |
| CS4 |  |  |  |
| CS5 |  |  |  |

| | **SET1: D = +20 oF of quencher outlet temperature** | | |
|---|---|---|---|
| | rH2 | CH4 in Separator vapor | CH4 in Mixture outlet |
| CS1 |  |  |  |
| CS2 |  |  |  |
| CS3 |  |  |  |
| CS4 |  |  |  |
| CS5 |  |  |  |

| | SET1: D = +0.05 methane mole fraction of FFGAS | | |
|---|---|---|---|
| | Tquen | Trin | Psep |
| CS1 |  |  |  |
| CS2 |  |  |  |
| CS3 |  |  |  |
| CS4 |  |  |  |
| CS5 |  |  |  |

|  | **SET1: D = +0.05 methane mole fraction of FFGAS** |  |  |
|---|---|---|---|
|  | rH2 | CH4 in Separator vapor | CH4 in Mixture outlet |
| CS1 |  |  |  |
| CS2 |  |  |  |
| CS3 |  |  |  |
| CS4 |  |  |  |
| CS5 |  |  |  |

| | **SET1: D = +0.05 methane mole fraction of FFGAS** | | |
|---|---|---|---|
| | Prin | FFH2 | Benzene product |
| CS1 |  |  |  |
| CS2 |  |  |  |
| CS3 |  |  |  |
| CS4 |  |  |  |
| CS5 |  |  |  |

# VITA

Miss Suchada Suntisrikomol was born in Nonthaburi on January 20, 1982. She graduated Bachelor Degree in Chemical Engineering from Prince of Songkla University in 2004. After that she studied for Master's degree in Chemical Engineering and joined Control and Systems Engineering research group at Chulalongkorn University in 2006.